An Efficient Algorithm for Enumerating Chordless Cycles and Chordless Paths

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Abstract. A chordless cycle (induced cycle) C of a graph is a cycle without any chord, meaning that there is no edge outside the cycle connecting two vertices of the cycle. A chordless path is defined similarly. In this paper, we consider the problems of enumerating chordless cycles/paths of a given graph G=(V,E), and propose algorithms taking O(|E|) time for each chordless cycle/path. In the existing studies, the problems had not been deeply studied in the theoretical computer science area, and no output polynomial time algorithm has been proposed. Our experiments showed that the computation time of our algorithms is constant per chordless cycle/path for non-dense random graphs and real-world graphs. They also show that the number of chordless cycles is much smaller than the number of cycles. We applied the algorithm to prediction of NMR (Nuclear Magnetic Resonance) spectra, and increased the accuracy of the prediction.

1 Introduction

Enumeration is a fundamental problem in computer science, and many algorithms have been proposed for many problems, such as cycles, paths, trees and cliques [5,8,10,12,13,17]. However, their application to real world problems has not been researched very much, due to the handling needed for the huge amount of and the high computational cost. However, this situation is now changing, thanks to the rapid increase in computational power, and the emergence of data centric science. For example, the enumeration of all substructures frequently appearing in a database, i.e., frequent pattern mining, has been intensively studied. This method is adopted for capturing the properties of databases, or for discovering new interesting knowledge in databases. Enumeration is necessary for such tasks because the objectives cannot be expressed well in mathematical terms. The use of good models helps reduce the amount of output, and the use of efficient algorithms enables huge databases to be more easily handled [9,1,11]. More specifically, introducing a threshold value for the frequency, which enables controlling the number of solutions. In such areas, minimal/maximal solutions are also enumerated to reduce the number of solutions. For example, enumerating all cliques is usually not practical while enumerating all maximal cliques, i.e. cliques included in no other cliques, is often practical [13,10]. In real-world sparse graphs, the number of maximal cliques is not exponential, so, even in large-scale graphs,

the maximal cliques can often be enumerated in a practically short time by a stand alone PC even for graphs with millions of vertices. However, the enumeration of maximum cliques, that have the maximum number of vertices among all cliques, is often not acceptable in practice, since the purpose of enumeration is to find all locally dense structures, and finding only maximum cliques will lose relatively small dense structures, thus it does not cover whole the data.

Paths and cycles are two of the most fundamental graph structures. They appear in many problems in computer science and are used for solving problems, such as optimizations (e.g. flow problems) and information retrieval (e.g. connectivity and movement of objects). Paths and cycles themselves are also used to model other objects. For example, in chemistry, the size and the fusing pattern of cycles in chemical graphs, representing chemical compounds, are considered to be essential structural attributes affecting on several important properties of chemical compounds, such as spectroscopic output, physical property, chemical reactivity, and biological activity.

For a path/cycle P, an edge connecting two vertices of P but not included in P is called a chord. A path/cycle without a chord is called a chordless path/cycle. Since a chordless cycle includes no other cycle as a vertex set, it is considered minimal. Thus, chordless cycles can be used to represent cyclic structures. For instance, the size and fusing pattern of chordless cycles in chemical graphs as well as other properties of chemical structures are taken into account when selecting data for prediction of nuclear magnetic resonance (NMR) chemical shift values[14]. Most chemical compounds contain cycles. In chemistry, the term 'ring' is used instead of 'cycle', for example a cycle consisting of 5 vertices is called 5-membered ring. Since the character of ring structures of chemical compounds is assumed to be important to study the nature of the structure-property relationships, the ring perception is one of classical questions [2,3,4,7] in the context of chemical informatics, so called chemoinformatics. Several kinds of ring structures, such as all rings and the smallest set of smallest ring (SSSR) are usually included in a basic dataset of chemical information. NMR chemical shift prediction is a successful case where the information about chordless cycles is employed to improve the accuracy of the prediction. The path/cycle enumeration is supposed to be useful also for analysis of network systems such as Web and social networks.

In this paper, we consider the problem of enumerating all chordless paths (resp., cycles) of the given graph. While optimization problems for paths and cycles have been studied well, their enumeration problems have not. This is because there are huge numbers of paths and cycles even in small graphs. However, we can reduce the numbers so that the problem becomes tractable by introducing the concept of chordless. The first path/cycle enumeration algorithm was proposed by Read and Tarjan in 1975[12]. Their algorithm takes as input a graph G = (V, E) and enumerates all cycles, or all paths connecting given vertices s and t, in O(|V| + |E|) time for each. The total computation time is O((|V| + |E|)N) where N is the number of output cycles/paths. Ferreira et al. [6] recently pro-

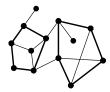


Fig. 1. Left bold cycle is a chordless cycle, right bold cycle has two chords.

posed a faster algorithm, that takes time linear in the output size, that is the sum of the lengths of the paths.

The chordless version was considered by Wild[19]. An algorithm based on the principle of exclusion is proposed, but the computational efficiency was not considered deeply. In this paper, we propose algorithms for enumerating chordless cycles and chordless paths connecting two vertices s and t (reported in 2003[18]). Note that chordless cycles can be enumerated by chordless path enumeration. The running time of the algorithm is O(|V|+|E|) for each, the same as the Read and Tarjan algorithm.

We experimentally evaluated the practical performance of the algorithms for random graphs and real-world graphs. The results showed that its practical computation time is much smaller than O(|V|+|E|), meaning that the algorithms can be used for large-scale graphs with non-huge amount of solutions. The results also showed that the number of chordless cycles is drastically small compared to the number of usual cycles.

2 Preliminaries

A graph is a combination of a vertex set and an edge set such that each edge is a pair of vertices. A graph G with vertex set V and edge set E is denoted by G = (V, E). An edge e of pair v and u is denoted by $\{u, v\}$. We say that the edge connects u and v, e is incident to u and v, and v and u are adjacent to each other, and call u and v end vertices of e. An edge with end vertices that are the same vertex is called a self-loop. Two edges having the same end vertices u and v are called multi-edges. We deal only with graphs with neither a self-loop nor a multi-edge. This restriction does not lose the generality of the problem formulation.

A path is a graph of vertices and edges composing a sequence $v_1, \{v_1, v_2\}, v_2, \{v_2, v_3\}, \ldots, \{v_{k-1}, v_k\}, v_k$ satisfying $v_i \neq v_j$ and $i \neq j$. The v_1 and v_k are called the end vertices of the path. If the end vertices of P are s and t, the path is called an s-t path. When $v_1 = v_k$ holds, a path is called a cycle. Here we represent paths and cycles by vertex sequences, such as (v_1, \ldots, v_k) . An edge connecting two vertices of a path/cycle P and not included in P is called a chord of P. A path/cycle P such that the graph includes no chord of P is called chordless. Figure 1 shows examples. In a set system composed of the vertex sets of cycles

(resp., s-t paths), the vertex set of a chordless cycle (resp., s-t path) is a minimal element.

For a graph G and a vertex subset S of G, $G \setminus S$ denotes the graph obtained from G by removing all vertices of S and all edges incident to some vertices in S. For a vertex v, N(v) denotes the neighbor of v, that is, the set of vertices adjacent to v. For a vertex set S and a vertex v, $S \setminus v$ and $S \cup v$ denote $S \setminus \{v\}$ and $S \cup \{v\}$, respectively. For a path P and its end vertex v, $P \setminus v$ denotes the path obtained by removing v from P.

Property 1. There is a chordless s-t path if and only if there is an s-t path.

Proof. A chordless s-t path is an s-t path, thus only if part is true. If an s-t path exists, a shortest path from s to t is a chordless s-t path, and thus it always exists.

Property 2. A vertex v is included in a cycle if and only if v is included in a chordless cycle.

Proof. If v is not included in any cycle, it obviously is not included in any chordless cycle. Hence, we investigate the case in which v is included in a cycle C. If C is chordless, we are done. If C has a chord, the addition of the chord splits C into two smaller cycles, and v is always included in one of them. We then consider the cycle as C. The cycle with three vertices can not have a chord, thus we always meet a chordless cycle including v.

For a recursive algorithm, an iteration means the computation from the beginning of a recursive call to its end, excluding any computation done in recursive calls generated in the iteration. If an iteration I recursively calls an iteration I', I' is called a *child* of I, and I is called the *parent* of I'.

3 Algorithm for Chordless s-t Path Enumeration

Our enumeration problem is formulated as follows.

Chordless s-t path enumeration problem

For a given graph G = (V, E) and two vertices s and t, enumerate all chordless s-t paths included in G.

We first observe that chordless cycle enumeration is done with chordless s-t path enumeration by repeating steps; (1) for a vertex s, enumerate chordless s-t paths in $G \setminus \{s,t\}$ for each vertex t adjacent to s, and (2) remove s from the graph. Here $G \setminus \{s,t\}$ is the graph obtained from G by removing the edge $\{s,t\}$. This implies that we only have to consider chordless s-t path enumeration.

Lemma 1. For a vertex $v \in N(s)$, P is a chordless s-t path including v if and only if $P \setminus s$ is a chordless v-t path of the graph $G \setminus (N(s) \setminus v)$.

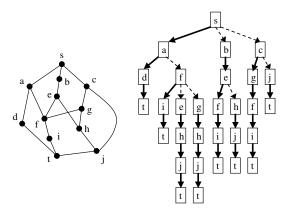


Fig. 2. Tree on the right represents recursive structure of *s-t* path enumeration in the graph on left; bold lines correspond to recursive calls in step 2, and dotted lines correspond to those in step 6.

Proof. If $P \setminus s$ is a chordless v-t path in $G \setminus (N(s) \setminus v)$, P is an s-t path all whose chords are incident to s. Since P has no vertex in $N(s) \setminus v$, no vertex of P other than v is adjacent to s. Thus, P has no chord incident to s, and is chordless.

If P is a chordless s-t path including v, no vertex $u \in N(s) \setminus v$ is included in P, since the edge $\{s, u\}$ would be a chord if was included. Thus, $P \setminus s$ is a chordless v-t path in $G \setminus (N(s) \setminus v)$.

Lemma 2. The set of chordless s-t paths of G is partitioned into disjoint sets of chordless s-t paths in the graphs $G \setminus (N(s) \setminus v)$ for each v.

Proof. Suppose that P is a chordless s-t path in G. Then, from lemma 1, P includes exactly one vertex among N(s). If P includes $v \in N(s)$, $P \setminus s$ is a chordless v-t path in $G \setminus (N(s) \setminus v)$, thus P is a chordless s-t path in $G \setminus (N(s) \setminus v)$. Since P is not an s-t path in $G \setminus (N(s) \setminus u)$ for any $u \in N(s) \setminus v$, the statement holds.

From the lemma, we obtain the following algorithm. The Q is the sequence of vertices attached to the paths in the ancestor iterations, and set to be empty at the start of the algorithm.

Enum_Chordless_Path (G = (V, E), s, t, Q)

- 1. if edge $\{s,t\}$ exists in E then output $Q \cup t$; return
- 2. for each $v \in N(s)$ s.t. a v-t path exists in $G \setminus (N(s) \setminus v)$ do
- 3. call Enum_Chordless_Path $((G \setminus (N(s) \setminus v)) \setminus s, v, t, Q \cup v)$
- 4. end for

When a recursive call is generated in an iteration of the algorithm, $G \setminus (N(s) \setminus v)$ is generated from G by removing vertices and edges. The removed vertices and edges are kept in memory so that G can be reconstructed from the graph. A removed edge or vertex is not removed again in the descendants of the iteration. Thus, the accumulated memory usage for these removed vertices and edges is O(|V| + |E|), and the space complexity of the algorithm is O(|V| + |E|).

In step 2, all vertices $v \in N(s)$ such that a v-t path exists in $G \setminus (N(s) \setminus v)$ must be listed. If and only if the condition in step 2 holds, there is a vertex $u \in N(v)$ such that a u-t path exists in $(G \setminus N(s)) \setminus s$. Thus, those vertices can be listed by computing the connected component including t in $G \setminus N(s) \setminus s$ and checking the condition in step 2 for all $u \in N(v)$ for all $v \in N(s)$. This can be done in O(|V| + |E|) time. The construction of $(G \setminus (N(s) \setminus v)) \setminus s$ is done in O(|N(v)|) time by constructing it from $(G \setminus N(s)) \setminus s$. Therefore, the time complexity of an iteration is O(|V| + |E|).

Let us consider the recursion tree of the algorithm which is a tree representing the recursive structure of the algorithm. The vertex of the recursion tree corresponds to an iteration, and each iteration and its parent are connected by an edge. The leaves correspond to the iterations generating no recursive calls, and the algorithm outputs a solution on each leaf. Because of the condition given placed on vertices in step 2, there is always at least one s-t path in the given graph. This implies that at least one recursive call occurs when step 2 is executed. Hence, the algorithm outputs a solution at every leaf of the recursion tree. The depth of the recursion tree is O(|V|) since at least one vertex is removed from the graph to generate a recursive call. We can conclude from these observations that the time complexity of the algorithm is O(N|V|(|V|+|E|)) where N is the number of chordless s-t paths in G. Next, we discuss the reduction of the time complexity to O(N(|V|+|E|)).

We first rewrite the above algorithm as follows. We denote the vertex next to v in path P by nxt(v). Note that although we introduce several variables, the algorithms are equivalent.

```
Enum_Chordless_Path2 (G = (V, E), s, t, Q)

1. if s is adjacent to t then output Q \cup t; return

2. P := a chordless s-t path in G

3. call Enum_Chordless_Path2 (G \setminus (N(s) \setminus nxt(s)), nxt(s), t, Q \cup nxt(s))

4. for each v \in N(s), v \neq nxt(s) do

5. if there is a v-t path in G \setminus (N(s) \setminus v) then

6. call Enum_Chordless_Path2 (G \setminus (N(s) \setminus v), v, t, Q \cup v)

7. end for
```

We further rewrite the algorithm as follows. We compute the chordless s-t path P computed in step 2 of the above algorithm, before the start of the
iteration, i.e., in its parent, and give it as a parameter to the recursive call.

```
Enum_Chordless_Path3 (G = (V, E), s, t, Q, P)
1. if s is adjacent to t then output Q \cup t; return
2. call Enum_Chordless_Path3 (G \setminus (N(s) \setminus nxt(s)), nxt(s), t, Q \cup nxt(s), P \setminus s)
3. for each v \in N(s), v \neq nxt(s) do
4. if there is an v-t path in G \setminus (N(s) \setminus v) then
5. P := a chordless v-t path in G \setminus (N(s) \setminus v) (found by a breadth first search)
6. call Enum_Chordless_Path3 (G \setminus (N(s) \setminus v), v, t, Q \cup v, P)
7. end if
8. end for
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Figure 2 illustrates an example of the recursive structure of this algorithm. The tail of an arrow is a parent and the head is its child. We call the child generated in step 2 first child, and the arrow pointing at the first child is drawn with a bold line. We can make a path by following the bold-arrows, and we call a maximal such path a straight path. Since the bottom of a straight path is a leaf, the number of straight paths is bounded by the number of chordless paths. Since the head of a non-bold arrow always points an end of a straight path, the number of non-bold arrows, that correspond to the recursive calls done in step 6, is bounded by the number of straight paths.

From these observations, we infer the following points regarding time complexity.

- An iteration takes O(|V| + |E|) time when a chordless path is output. This computation time is O(|V| + |E|) per chordless path.
- Steps 1 and 2 take O(NN(s)) time where NN(s) is the number of edges adjacent to vertices in N(s). This time is spent checking the adjacency of s and t and constructing $G \setminus (N(s) \setminus v)$ for all $v \in N(s)$. This comes from that $G \setminus (N(s) \setminus v)$ can be constructed from $G \setminus N(s)$ by adding edges adjacent to v in O(|N(v)|) time.
- The number of executions of the for loop in step 3 is bounded by |N(s)|. Their sum over all iterations in a straight path does not exceed the number of edges.
- Steps 5 and 6 take O(|V| + |E|) time to find a chordless v-t path, and to construct $G \setminus (N(s) \setminus v)$. Since the recursive call in step 6 corresponds to a straight path, this computation time is O(|V| + |E|) per chordless path.
- The execution time for step 4 is O(|V| + |E|).

We see from the above that the bottle neck in terms of time complexity is step 4. The other parts of the algorithm takes O(|V| + |E|) time per chordless s-t path. We speed up step 4 by using the following property.

Property 3. $G \setminus \{v\}$ includes a v-t path for $v \in N(s)$ if and only if there is a vertex $u \in N(v) \setminus N(s)$ such that $G \setminus N(s)$ includes a u-t path. \square

In each iteration we put mark on vertices u such that there is a u-t path in $G \setminus N(s)$. Step 4 is then done in O(|N(v)|) time by looking at the marks on the vertices in N(v). The marks can be put in short time, by updating the marks put in the first child. The condition of step 4 is checked by finding all vertices in $G \setminus N(s)$ from which going to t is possible. This also takes O(|V| + |E|) time, but the time is reduced by re-using the results of the computation done for the first child. In the first child, marks are put according to the reachability to t in $G \setminus (N(s) \cup N(nxt(s)))$. To put marks for $G \setminus N(s)$, we find all vertices u such that any u-t path in $G \setminus N(s)$ includes a vertex of $N(nxt(s)) \setminus N(s)$. This is done by using a graph search starting from the vertices of $N(nxt(s)) \setminus N(s)$ that are adjacent to a marked vertex, and visiting only unmarked vertices. The time taken is linear in the number of edges adjacent to newly marked vertices.

Consider the computation time with respect to step 4, for the iterations in a straight path. In these operations, a vertex (resp., an edge) gets a mark at most

once, i.e., it never gets a mark twice. Thus, the total computation time for this computation is linear in the sum of the degrees of marked vertices and vertices in N(nxt(s)), and is bounded by O(|V|+|E|). The computation time for step 4 is thus reduced to O(|V|+|E|) per chordless s-t path. When a recursive call for a non-first child is made, all marks are deleted. We then perform a graph search starting from t to put the marks. Both steps take O(|V|+|E|) time. Since this computation is done only when generating non-first child, the total number of occurrences of this computation is bounded by the number of maximal paths, i.e., the number of chordless paths. Thus, this computation takes O(|V|+|E|) time for each chordless path. The algorithm is written as follows.

```
Enum_Chordless_Path4 (G = (V, E), s, t, Q, P)
1. if s is adjacent to t then output Q \cup t; go to 11
2. call Enum_Chordless_Path4 (G \setminus (N(s) \setminus nxt(s)), nxt(s), t, Q \cup nxt(s), P \setminus s)
3. put mark by graph search on G \setminus N(s) from vertices in N(nxt(s))
4. for each v \in N(s), v \neq nxt(s) do
4. if a vertex adjacent to v is marked then
5. delete marks from all vertices in G
6. P := a chordless v-t path in G \setminus (N(s) \setminus v)
7. call Enum_Chordless_Path4 (G \setminus (N(s) \setminus v), v, t, Q \cup v, P)
8. recover the marks deleted in step 5, by graph search starting from t on G \setminus N(s)
9. end if
10. end for
```

Theorem 1. The chordless s-t paths in a given graph G = (V, E) can be enumerated in O(|V| + |E|) time per chordless path, in particular, polynomial time delay.

Proof. We can see the correctness in the above. The time complexity of an iteration is O(|V| + |E|), and each iteration outputs an s-t-path. Moreover, the height of the recursion tree is at most |V|, thus the time between two consecutive output paths is bounded by O(|V| + |E|) + O(|V|) = O(|V| + |E|). This concludes the theorem.

Theorem 2. The chordless cycles in a given graph G = (V, E) can be enumerated in O(|V| + |E|) time per chordless cycle, in particular, polynomial time delay.

4 Computational Experiments

The practical efficiency of the proposed algorithms is evaluated by computational experiments. The results were compared with those of the cycle enumeration algorithm proposed in [12]. The difference between the number of cycles and of chordless cycles was also compared. The program was coded in C, and compiled using gcc. The experiments were done on a PC with a Core i7 3GHz CPU. The

Table 1. Computational time (in seconds) for randomly generated graphs

edge density	10%	20%	30%	40%	50%	60%	70%	80%	90%
no. of vertices 50	0.18	0.12	0.098	0.089	0.082	0.08	0.085	0.1	0.11
75	0.17	0.12	0.099	0.088	0.079	0.074	0.077	0.088	0.1
100	0.17	0.12	0.099	0.09	0.083	0.081	0.089	0.095	0.12
150	0.2	0.12	0.099	0.098	0.077	0.075	0.083	0.103	0.14
200	0.18	0.12	0.1	0.088	0.081	0.078	0.085	0.11	0.17
300	0.19	0.12	0.1	0.087	0.082	0.083	0.091	0.12	0.21
400	0.17	0.12	0.1	0.089	0.08	0.086	0.1	0.15	0.26
600	0.18	0.11	0.12	0.12	0.11	0.1	0.13	0.23	0.42
800	0.2	0.12	0.14	0.13	0.11	0.11	0.13	0.26	0.54
1200	0.23	0.17	0.17	0.13	0.12	0.12	0.15	0.28	1
1600	0.24	0.19	0.14	0.13	0.13	0.14	0.21	0.29	1.3
2400	0.25	0.19	0.17	0.15	0.16	0.16	0.19	0.44	1.4
3200	0.29	0.23	0.2	0.19	0.18	0.2	0.25	0.61	1.79
4800	0.28	0.28	0.27						

code is available at the author's web site (http://research.nii.ac.jp/ũno/codes.html). We did not use multiple cores, and the memory usage was less than 4MB. The instance graphs were random graphs and the real-world graphs taken from the UCI machine learning repository[16]. All the test instances shown here are downloadable from the author's web site, except for those from UCI repository. Tables 1 to 4 summarize the computation time, number of cycles, and number of chordless cycles for each instance, and clarify the effectiveness of the chordless cycle model and our algorithm.

The computation time results for randomly generated graphs are shown in Table 1. The edge density means the probability of being connected by an edge for any two vertices. Execution of an enumeration algorithm involves many iterations with different input graphs, thus we thought that there are sufficiently many samples even in one execution of the algorithm. Therefore, we generated just one instance for each parameter. Each cell represents the computation time needed for 10,000 cycles or chordless cycles. When the computation time was too long so that the number of output cycles exceeded one million, we stopped the computation.

When the edge density was close to 100%, almost all the chordless cycles were triangles. In this case, intuitively, the algorithm spent $O(|V||E|) = O(|V|^3)$ time to find $O(|V|^2)$ chordless cycles. In contrast, it took almost constant time for each chordless cycle in sparse graphs. This is because the graph was reduced by repeated recursive calls, and at the bottom levels, the graph sizes were usually constant.

Table 2 shows that the number of chordless cycles exponentially increased against with the edge density, but not as much as usual cycles. Table 3 shows the experimental results for sparse graphs. The graphs were generated by adding chords randomly to a cycle of n vertices so that the average degree was four. These sparse graphs included so many chordless cycles. The graphs with at most

Table 2. Number of chordless cycles (upper) and of cycles (lower)

edge density	10%	20%	30%	40%	50%	60%	70%	80%	90%	100%
no. of vertices 10	1	3	14	20	41	45	63	81	120	
	0	1	4	116	352	2302	3697	24k	108k	
15	0	10	34	116	165	193	247	297	350	455
	0	36	1470	613k	6620k	55525k	-	-	-	-
20	1	78	298	523	637	752	771	846	908	1140
	1	56k	9114k	-	-	-	-	-	-	-
25	8	1218	2049	2387	2099	1891	1775	1854	1928	2300
50	64k	395k	267k	146k	82k	49k	34k	23k	18k	19k
75	119379k	69357k	14504k	3679k	1158k	465k	221k	119k	73810	67525
100	-	-	-	40436k	8269k	2395k	877k	393k	199k	161k
150	-	-	-	-	149022k	27483k	6641k	2167k	854k	551k
200	-	-	-	-	-	167408k	30334k	7755k	2466k	1313k
300	-	-	-	-	-	-	-	51043k	11457k	4455k
400	-	-	-	-	_	-	_	-	35154k	10586k

Table 3. Computation time and number of chordless cycles for sparse graphs

graph size (no. of vertices)	10	20	30	40	50	60	70	80	90
no. of chordless cycles	12	90	743	5371	89164	853704	4194491	45634757	-
time for $10,000$ chordless cycles	16.6	3.33	0.53	0.22	0.18	0.2	0.23	0.24	-

100 vertices were solved in a practically short time, and the computation time for each chordless cycle were almost the same.

Table 4 shows the number of chordless cycles with limited lengths including a vertex (the first vertex) for the real-world data, taken from the UCI repository. The number of all chordless cycles is shown at the bottom for reference. The graphs were basically sparse, and globally well connected, and thus included a large number of cycles. Even in such cases, by giving an upper bound of the length, Some graphs can be made tractable in such cases by placing an upper bound on the length. These results show the possibility of using chordless cycles with limited lengths for practical data analysis of real-world graphs such as those for social networks.

4.1 Application to NMR Prediction

Chordless cycle enumeration has already been implemented as a part of a database system of chemoinformatics[14], composed of structural data of chemical compounds. In this system, the number of chordless cycles in the chemical graph of a chemical compound is considered to be an attribute of the compound. In response to a query about the chemical structure of a compound, the system searches in the database for structures partially similar to the structure of query compound, and predict some functions of the query compound. A chemical graph is usually sparse and is globally a tree or a combination of several large cycles.

Table 4. No. of chordless cycles including a vertex (of ID 0), for real-world graphs

	adjnoun	astro-ph	breast	celegen	cond-mat-20	005 cond	mat_large	dolphins
(no. of vertices)	114	16708	7539	298	404	123	30561	64
(no. of edges)	425	121251	5848	2359	1756	693	24334	159
length < 5	8	327	-	3342	5	393	6	26
length < 8	251		-	1738k		-	6	320
length < 16	65350	-	-	-		-	6	1780
#chord. cyc.	66235k	-	-	-		-	-	6966
	football	human_p	pi kara	te lesmi	s netscience	polblogs	polboopks	power
(no. of vertices)	football 117	human_p			s netscience 9 1591	polblogs 1492	polboopks	
(no. of vertices) (no. of edges)		1034	47		9 1591		107	4943
	117 616	1034	47 18	36 7 78 25	9 1591	1492	107	4943 6594
(no. of edges)	117 616 81	1034 541	47 18 38	36 7 78 25 37	9 1591 4 2742	1492 19090	107 441	4943 6594
$\frac{\text{(no. of edges)}}{\text{length}} < 5$	117 616 81 11869	1034 541 183	47 18 38 -	36 7 78 25 37 38	9 1591 4 2742 3 1	1492 19090	107 441 21	4943 6594 0 7 4

Small components can be attached to the large cycles. Thus, the number of chordless cycles is not so huge and is tractable in most cases.

The program code was implemented in the CAST/CNMR system for predicting the ¹³C-NMR chemical shift[14,15]. The codes and a more precise description of this system are available at http://research.nii.ac.jp/hsatoh/subjects/NMR-e.html. The information obtained about chordless cycles is used to improve the accuracy for the predicted values when the ring attributes affects the NMR spectrum. The CAST/CNMR system predicts chemical shifts by using a chemical structure-spectrum database, containing mainly natural organic products and their related synthetic compounds. Since most of the compounds include chains of fused rings, enumerating all rings for these compounds would greatly increase the output size, with lots of data useless for NMR prediction. Therefore, the chordless cycle was adopted as a relevant ring attribute for the CAST/CNMR system. For accurate NMR prediction for carbon atoms, an error within 1.0 ppm (parts per million) is generally required. Use of chordless cycle information reduced error values of -4.1 to 1.6 ppm for some problematic carbon atoms to less than 1.0 ppm[14].

5 Conclusion

We proposed an algorithm for enumerating all chordless s-t paths, that is applicable to chordless cycle enumeration without increasing the time complexity. By reusing the results of the subroutines, the computation time is reduced to O(|V| + |E|) for each chordless path. The results of the computational experiments showed that the algorithm works well for both random graphs and real-world graphs; the computation time was O(|V|) in dense graphs, and almost constant for sparse graphs. The results also showed that the number of chord-

less cycles is small compared to the number of usual cycles. This algorithm thus paves the way to efficient use of cycle enumeration in data mining.

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