## Department of Computer Science <br> Technical Report

# Implementation of an Automated <br> Proof for an Algorithm Solving the Maximum Independent Set Problem 

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# Implementation of an Automated Proof for an Algorithm Solving the Maximum Independent Set Problem 

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#### Abstract

Kneis, Langer, and Rossmanith [3] proposed an algorithm that solves the maximum independent set problem for graphs with $n$ vertices in $\mathcal{O}^{*}\left(1.2132^{n}\right)$. This bound is obtained by precisely analyzing all cases that the algorithm may encounter during execution. Since the number of cases exceeds several millions, a computer aided proof is used to generate and evaluate all cases. In this paper, we present a program that fullfills this task and give a detailed description of the principles underlying our method. Moreover, we prove that the set of generated cases includes all relevant cases.


## 1 Motivation

The Maximum Independent Set problem (Mis) is well known to be NP-hard. Over the past years, several exact algorithms were developed for this problem. Tarjan and Trojanowski [7] presented a method to solve it in time $O^{*}\left(1.261^{n}\right)$. This was improved by Jian [4] to $O^{*}(1.235)$ and by Robson [6] to $\left.O^{*}(1.228)^{n}\right)$. In 2006, Fomin, Grandoni and Kratsch [2] devised a new algorithm with a runtime bounded by $O^{*}\left(1.2201^{n}\right)$.

Recently, Kneis, Langer, and Rossmanith [3] developed an intuitive algorithm that solves Mis in time $\mathcal{O}^{*}\left(1.2132^{n}\right)$. To prove this new runtime bound, however, a computer aided case distinction was applied. The number of these cases, however, is extremely large and hence demands for an efficient generation method are justified. In this paper we present an implementation of this proof and give a detailed documentation.

Throughout this paper we will try to convey an intuitive understanding of our method and subsequently analyze all involved steps in detail. Finally we will give a formal proof that our method generates the cases relevant for [3].

## 2 Definitions

Since this report is intended to complement the proof in [3], we will only shortly repeat the relevant definitions here.

Definition 1 ([3]). Let $H=\left(V_{I} \cup V_{O}, E\right)$ be graph, such that $V_{I} \cap V_{O}=\emptyset$, and let $v \in V_{I}$ such that $V_{I}=N^{i}[v], V_{O}=N^{i+1}(v)$ and $\operatorname{deg}(u)=1$ for $u \in V_{O}$. Moreover, let $\operatorname{deg}(v) \geq \operatorname{deg}(u)$ for all $u \in V_{I} \cup V_{O}$. We call $(H, v)$ graphlet of radius $i$. We call $V_{I}$ the inner vertices of $(H, v)$ and the set of edges between $V_{I}$ and $V_{O}$ the anonymous edges.

Definition 2. Let $(G, v)$ be a graphlet. The $k$-th orbit $O_{k}$ is defined by $O_{k}=$ $\{u \in V(G) \mid d(u, v)=k\}$ where $d(\cdot, \cdot)$ is the distance.

Definition 3. Let $(G, v)$ be a graphlet. $(G, v)$ has extent $n \in \mathbb{N}$ if and only if $O_{n} \neq \emptyset$ and $O_{n+1}=\emptyset$.

Definition 4. Let $(G, v)$ and $\left(G^{\prime}, v^{\prime}\right)$ be graphlets with vertex sets $V_{I}, V_{O}$ and $V_{I}^{\prime}$, $V_{O}^{\prime}$ respectively. A bijective mapping $\pi: V(G) \rightarrow V\left(G^{\prime}\right)$ is a graphlet isomorphism if and only if $\pi$ is an isomorphism w.r.t. $G$ and $G^{\prime}$ and additionally $\pi(v)=v^{\prime}, \pi\left(V_{I}\right)=V_{I}^{\prime}$ and $\pi\left(V_{O}\right)=V_{O}^{\prime}$. If such a mapping exists, we write $(G, v) \cong\left(G^{\prime}, v^{\prime}\right)$.

Terms surrounded by < and > refer to command line parameters used when invoking scripts or programs; identifiers surrounded by [ and ] refer to program names.

## 3 Generation

Throughout this section we will give a rough overview of our graphlet generation method. Afterwards, we will investigate the steps occurring in the generation algorithm in more detail.

In the first subsection we will specify some properties of the relevant cases. We exploit these properties in order to generate the relevant cases more efficiently. In the subsequent subsections we will discuss the relevant parameters used to setup the generation process.

### 3.1 Relevant cases

By the proof given in [3] we know that all cases the algorithm considers for branching are fully reduced. Moreover, Theorem 3 from this paper allows us to restrict the relevant cases to graphlets with the following properties:

- $d(u) \geq 3$ holds for all $u \in V(G)$, since vertices of degree smaller or equal 2 are removed by the domination- and folding-rule.
- There is no $u \in O_{1}$, such that $u$ has no neighbor in $O_{2}$, since in this case $v$ would dominate $u$.
- There is no $u \in V(G)$, such that $d(u)>d(v)$, since the algorithm always branches on a vertex of maximum degree and we assume that $v$ is the vertex on which the algorithm branches.
$-d(v)=4$.
- $(G, v)$ has radius 2.
- Since Kneis, Langer, and Rossmanith showed that, for a case where $\left|O_{2}\right| \geq$ 8, the algorithm's performance is sufficient, the generated cases comply to $\left|O_{2}\right| \leq 7$.

Therefore our objective boils down to: Generate all graphlets $(G, v)$ with radius 2 and $d(v)=4$, where $d(u) \in\{3,4\}$ for all vertices $u \in V(G),\left|O_{2}\right| \leq 7$ and all vertices in $O_{1}$ have at least one neighbor in $O_{2}$.

### 3.2 Parameters

The behaviour and output of the generation algorithm are modified by three mandatory parameters <minDegree>, <maxDegree>, and <extent>. Because of the restrictions above the <extent> is already fixed at 2 and therefore hardcoded in the program.

The <minDegree> and <maxDegree> specify the minimum and maximum degree that any vertex in the generated cases may have. The algorithm by Kneis, Langer, and Rossmanith branches on graphlets which do not have vertices of degree 1 or 2 . Therefore <minDegree> is set to 3 . Since cases with $d(v) \geq 5$ where investigated manually, we only need to generate graphlets with a <maxDegree> of 4 .

### 3.3 Process overview

Listing 1.1 visualizes the steps used to generate the relevant cases. We describe the applied steps in a succinct manner. Afterwards, however, we give detailed information on the effect and implementation of the steps.

Listing 1.1. Process overview in pseudo-code.

```
generateStars(minDegree, maxDegree)
makeIntraOrbit1Edges(minDegree, maxDegree)
pickRepresentatives()
appendTrees(minDegree, maxDegree)
foldLeaves (maxDegree)
pickRepresentatives()
makeIntraOrbit2Edges(minDegree, maxDegree)
pickRepresentatives()
appendAnonymousEdges(minDegree, maxDegree)
```

1. We initially invoke generateStars (minDegree, maxDegree). This generates a set $\mathcal{S}$ of star-shaped graphlets. These are all graphlets $(G, v)$ with extent 1 , where $d(v) \in\{$ minDegree, $\ldots$, maxDegree $\}$ and that do not contain any edges between vertices in $O_{1}$ (cf. Figure 2).
2. The invocation of makeIntraOrbit1Edges (minDegree, maxDegree) generates all relevant graphlets by connecting vertices in the first orbit of the graphlets in $\mathcal{S}$ from the previous step.
3. Afterwards, the pickRepresentatives () step is applied for the first time. In this step we determine the isomorphy classes in the set of graphlets generated so far. Then we choose one representative from each class and continue to work on these representatives only, thus reducing the number of graphlets processed further.
4. The call to appendTrees (minDegree, maxDegree) generates graphlets by appending new vertices to the vertices on the highest orbit of each graphlet generated so far. This step generates all possible graphlets of extent two, where each vertex in $O_{2}$ has exactly one neighbor in $O_{1}$ and no further incident edges. Moreover, minDegree $\leq \operatorname{deg}(u) \leq \operatorname{maxDegree}$ for all $u \in O_{1}$ still holds after this step.
5. In the next step, the foldLeaves (maxDegree), the new vertices from step 4 are merged with each other in all possible ways. Doing so, we generate all graphlets of extent two such that $G\left[O_{2}\right]$ contains no edges and without any anonymous edges. This step provides a very inexpensive method of pruning the search-tree (cf. Section 3.4).
6. The invocation of makeIntraOrbit2Edges(minDegree, maxDegree) has the same effect as makeIntraOrbit1Edges (minDegree, maxDegree), but on $\mathrm{O}_{2}$ instead of $O_{1}$. Hence, this step generates all graphlets of extent two without anonymous edges.
7. Finally, we add all possible valid combinations of anonymous edges, by calling appendAnonymousEdges(minDegree, maxDegree).

Depending on the used parameters, the memory consumption of the procedure easily exceeds the resources of a conventional computer. Therefore, we made extensive use of disk storage: Between each two steps the intermediate results are stored on the hard-drive. This of course is a major performance penalty, but the obtained runtimes for our scenario were more than acceptable. Listing 1.2 shows the actual script that is used to coordinate the generation of the relevant cases. The steps described above are implemented as autonomous programs which work on sets of graphlets stored on the disk.

Listing 1.2. The script coordinating the generation process.

```
. / sinit \(-\mathrm{m}=\$ 1-\mathrm{M}=\$ 1-\mathrm{o}=\) stage \(1 /\) init
./sedge \(-\mathrm{i}=\) stage \(1-\mathrm{o}=\) stage \(2-\mathrm{M}=\$ 1\)
cd stage2/
for N in \(*\); do
../shash \(-\mathrm{i}=\$ \mathrm{~N}-\mathrm{o}=. . /\) stage \(3 /\)
done
cd . .
cd stage3/
for N in \(*\); do
.. \(/\) sfindiso \(-i=\$ N-r=\$ N . r-t=10000\)
\(\ldots /\) sclean \(-\mathrm{i}=\$ \mathrm{~N}-\mathrm{r}=\$ \mathrm{~N} . \mathrm{r}-\mathrm{o}=. . /\) stage \(4 / \$ \mathrm{~N}\)
done
cd . .
./smerge \(-\mathrm{i}=\) stage \(4 /-\mathrm{o}=\) stage \(5 /\) set
. / sexpand \(-\mathrm{i}=\) stage \(5 /\) set \(-\mathrm{o}=\) stage \(6 /\) set \(-\mathrm{m}=\$ 2-\mathrm{M}=\$ 1\)
./sfold \(-\mathrm{i}=\) stage \(6 /\) set \(-\mathrm{o}=\) stage \(7 /\)
cd stage7/
for N in \(*\); do
../shash \(-\mathrm{i}=\$ \mathrm{~N}-\mathrm{o}=. . /\) stage \(8 /\)
done
cd ..
cd stage8/
for N in *; do
    . / sfindiso \(-\mathrm{i}=\$ \mathrm{~N}-\mathrm{r}=\$ \mathrm{~N} . \mathrm{r}-\mathrm{t}=1000\)
    ../sclean \(-\mathrm{i}=\$ \mathrm{~N}-\mathrm{r}=\$ \mathrm{~N} . \mathrm{r}-\mathrm{o}=. . /\) stage \(9 / \$ \mathrm{~N}\)
done
cd ..
. sedge \(-\mathrm{i}=\) stage \(9-\mathrm{o}=\) stage \(10-\mathrm{M}=\$ 1\)
cd stage10/
```

```
for N in *; do
../shash - i=$N -o=../stage11/
done
cd ..
cd stage11/
for N in *; do
../ sfindiso - i=$N - r=$N.r -t=10000
../sclean -i=$N - r=$N.r -o=_/stage12/$N
done
cd ..
./smerge }-\textrm{i}=\mathrm{ stage12/ -o=stage13/set
./ sanon - i=stage13/set -o=output/$1-$1.$2-$1.$3-$1 -m=$3 -M=$1
```

Furthermore, the pickRepresentatives() function is split into three programs (shash, sfindiso, sclean). Note that checking for isomorphisms is absolutely necessary to restrict the number of generated graphlets. Since an exhaustive check is very expensive, we only compare graphlets with the same hash value (see Section 4). This step improves the performance of the generation process dramatically.

### 3.4 Process sequence

As depicted in Section 3.3, the process consists of several autonomous programs. The programs' usage and implementations are elaborated throughout the next pages. This part of the report is intended to serve as a guideline to understand the programs' implementations, as well as a manual on how to use them.
generateStars(minDegree, maxDegree) [sinit] The invocation of sinit requires certain parameters (cf. Listing 1.3). For every <m> $\leq n \leq<M>$ an $n$ Star graphlet is generated and stored in the file <o>, where an $n$-Star is defined as a grahplet $(G, v), G=\left(\{v\} \cup O_{1}, E\right)$ with $O_{1}=\left\{u_{1}, \ldots, u_{n}\right\}$ and $E=\left\{\left\{v, u_{1}\right\}, \ldots,\left\{v, u_{n}\right\}\right\}$.

Listing 1.3. Invocation syntax for sinit.

```
Invocation: sinit [OPTIONS]
Generates a set of initial graphs for the generation process.
    -m, --mindegree Specifies the minimum degree of the anchor
    -M, -maxdegree Specifies the maximum degree of the anchor
    -o, --output Selects the output file (defaults to 'init.out')
```

makeIntraOrbit $\{\mathbf{1}, \mathbf{2}\}$ Edges (minDegree, maxDegree) [sedge] The invocation of sedge requires three parameters, as described in Listing 1.5.

Let $S$ be the set of graphlets with extent $i$. For any $(G, v) \in S$, all $x, y \in O_{i}$ are - by construction - not adjacent, cf. Listings 1.1 and 1.2. Our goal is now to add all possible sets of edges inside $O_{i}$ to these graphes (see Figure 1). Note that the extent $i$ of a given graphlet is determined automatically by the algorithm.

For this purpose we compute a list $L$ of pairs of vertices whose degree is strictly less than the degree of the anchor vertex. These are exactly the pairs of
vertices which we may connect without violating the maximal degree restrictions:

$$
L=\{\{x, y\} \mid d(x)<d(v) \wedge d(y)<d(v)\}
$$

The algorithm's behaviour is a simple (exhaustive) search for all possibilities, as depicted in Listing 1.4. In Line 7, however, we need to update the candidate list $L$, since adding edges might disqualify certain pairs.


Fig. 1. Constructing edges in $O_{1}$ of a 3 -star.

Listing 1.4. Sedge pseudo-code.

```
For all (G,v) in the input file do {
    L}=\mathrm{ computeCandidates ()
    addEdges((G,v), L)
}
addEdges((G,v), L) {
    updateList(L)
    if (isEmpty(L)) {
        writeToDisk(G,v)
        return.
    }
    {x,y} = firstElementOf(L)
    L
    /* Realize the edge */
    (G',}\textrm{v})=(\textrm{G},\textrm{v})\mathrm{ where E[G'] = E[G] + {x,y}
    addEdges((G',v), L')
    /* Do not realize the edge */
    addEdges((G,v), L')
}
```

Listing 1.5. Invocation syntax for sedge.

```
Invocation: sedge [OPTIONS]
Connects the orbital vertices of a set of graphs.
    -i, --input The graph collection to fold.
    -o, --output A file to store the connected graphs.
    -M, --maxdegree The maximum degree of each vertex.
```

appendTrees (minDegree, maxDegree) [sexpand] Calling sexpand requires four parameters. They are described in Listing 1.7.

Given a set of graphlets $S$ with extent 1 this step constructs a new set $S^{\prime}$ of graphlets with extent 2 as follows: for each graphlet $(G, v) \in S$, consider its outermost orbit $O_{1}=\left\{v_{1}, \ldots, v_{n}\right\}$. For every such vertex $v_{i} \in O_{1}$ we then calculate the set

$$
\left.n\left(v_{i}\right):=\{a \in \mathbb{N}|<\mathrm{m}\rangle \leq a \leq \min \{<\mathrm{M}\rangle, d(v)\}\right\}
$$

If, for example, $n\left(v_{i}\right)=\{2,3,4\}$, the vertex $v_{i}$ can have 2,3 or 4 neighbors in $O_{2}$ without $d\left(v_{i}\right)$ being smaller than $\langle\mathrm{m}\rangle$, or too high.

Using the graphlet $(G, v)$ and some choice $a_{i} \in n\left(v_{i}\right)$ for all $1 \leq i \leq n$ we create a new graphlet $\left(G^{\prime}, v\right)$ by attaching $a_{i}$ new vertices to the vertex $v_{i}$. Consider a graphlet $(G, v)$ such that $V(G)=\{v\}$. The expansions results for $<m\rangle=3$ and $\langle M\rangle=5$ are illustrated in Figure 2.


Fig. 2. Expanding a single vertex for $n(v)=\{3,4,5\}$.

Every possibility to choose the $a_{i}$ from the $n\left(v_{i}\right)$ yields a graphlet. The set of the graphlets obtained by using all possible choices for the $a_{i}$ are added to the set $S^{\prime} . S^{\prime}$ is used as input for the next step.

For implementation details refer to the pseudo code in Listing 1.6.
Listing 1.6. Sexpand pseudo-code.

```
For all (G,v) in the input file do {
    Let O = outerMostOrbit (G,v)
    expand((G,v),O)
}
expand((G,v), O) {
    if (isEmpty(O)) {
        writeToDisk(G,v)
        return.
    }
    u = firstElementOf(O)
    for all i in n(u) do {
        (G',v) = appendFreshVertices(i, u, (G,v))
        expand ((G', v), O - u)
    }
}
```

In line 14 the new graphlet $\left(G^{\prime}, v\right)$ is obtained for some vertex $u$ and some choice $i \in n(u)$ by
$V\left(G^{\prime}\right)=V(G) \cup \dot{\cup}\left\{v_{1}, \ldots, v_{|n(u)|}\right\}$ and $E\left(G^{\prime}\right)=E(G) \cup\left\{\left\{u, v_{1}\right\}, \ldots,\left\{u, v_{|n(u)|}\right\}\right\}$

Listing 1.7. Invocation syntax for sexpand.

```
Invocation: sexpand [OPTIONS]
Expands a set of graphs by appending new vertices to the outermost
orbit.
    -i, --input The graph collection to expand.
    -o, --output The desired output-file.
    -m, --mindegree The minimum degree of a vertex.
    -M, --maxdegree The maximum degree of a vertex.
```

foldLeaves (maxDegree) [sfold] The invocation of sfold requires two parameters, as depicted in Listing 1.9.

Let $S$ be a set of graphlets of extent $k+1 \in \mathbb{N}$ generated by the sexpand program. Obviously there is no graphlet in $S$ such that two vertices in $O_{k}$ have a common neighbor in $O_{k+1}$ since for all $u \in O_{k+1}$ it holds $d(u)=1$. We then start to fold the vertices in the outermost orbit with each other.

Definition 5. Let $u, v \in O_{k+1}, u \neq v$ and $N(u) \cap N(v)=\emptyset$. We fold $u, v$ by introducing a new vertex $z$ and connecting it to all neighbors of $u, v$. Afterwards we delete $u, v$ from the graphlet.

For each graphlet $(G, v) \in S$ we start an exhaustive search on all possible ways to fold vertices in $O_{k+1}$. Refer to the following figure for an example.


Fig. 3. The graphlets obtained by folding vertices $u, v, w, x$ in the highest orbit in all possible ways (isomorphic graphs are omitted).

Listing 1.8. sfold pseudo-code.

```
For all (G,v) in the input file do {
    P}=\mathrm{ pairsOfVerticesInOutermostOrbit()
    foldVertices((G,v), P)
}
foldVertices((G,v), P) {
    updatePairs(P)
    if (isEmpty(P)) {
        writeToDisk(G, v)
        return.
    }
    {x,y} = firstElementOf(P)
    P
    /* Do not fold the vertices */
    foldVertices((G,v), P')
    /* Vertices foldable? */
    if (areDisjunctive(N(x), N(y))) {
        (G',v) = fold ((G,v), x, y)
        foldVertices((G',v), P')
    }
}
```

Note that the graphlet $\left(G^{\prime}, v\right)$ in Line 22 is obtained by performing the following steps:

1. Add a new vertex $u$ and remove the vertices $x, y: V\left(G^{\prime}\right)=(V(G) \dot{\cup}\{u\}) \backslash$ $\{x, y\}$.
2. Connect $u$ to all neighbors of $x, y:\{x, z\} \in E(G) \vee\{y, z\} \in E(G) \Rightarrow\{u, z\} \in$ $E\left(G^{\prime}\right)$.

The call to updatePairs (P) has two purposes. First it removes vertex pairs which cannot be folded anymore because either their neighborhoods now overlap or because of the removed vertices.

Second it creates new pairs for a new vertex - in case we applied folding in the previous round - and adds them to $P$.

Listing 1.9. Invocation syntax for sfold.

```
Invocation: sfold -i=input -o=output
Folds the orbital vertices of a set of graphs.
    -i, --input The graph collection to fold.
    -o, --output A file to store the folded graphs.
```

pickRepresentatives() [shash,sfindiso,sclean] The objective of these three programs is to pick representative graphlets from the present isomorphy classes. As a first step the shash program splits the present files into several new files. The file that a graphlet is saved to depends on its hash value (cf. Section 4).

Afterwards, exploiting that $(G, v) \cong\left(G^{\prime}, v^{\prime}\right) \Rightarrow h(G, v)=h\left(G^{\prime}, v^{\prime}\right)$, the sfindiso program searches for isomorphic graphlets, one file at a time, using a straightforward isomorphism checking algorithm. Finally the sclean program removes all members of an isomorphism class except for one representative.

Listing 1.10. Invocation syntax for shash.

```
Invocation: shash [OPTIONS]
Splits a set according to the hash value of each graph.
    -i, --input The input file.
    -o, --output A file to store the hash files.
```

Listing 1.11. Invocation syntax for sfindiso.

```
Invocation: sfindiso [OPTIONS]
Locates pairs of isomorphic graphs and writes their index into a file.
    -i, --input The graph collection to search.
    -r, --report A file to report the located isomorphisms to.
    -T, --time A global time limit. After this time has passed,
        the tool stops looking for isomorphic graphs.
        The number of non-deterministic steps the
        isomorphism checking algorithm is limited to for
        each pair of graphs.
-o, --offset The index of the first graph to check.
```

Listing 1.12. Invocation syntax for sclean.

```
Invocation: sclean [OPTIONS]
Locates pairs of isomorphic graphs and writes their index into a
file.
    -i, --input }\quad\mathrm{ The graph collection to clean.
```


## 4 Hashing function

Throughout the generation process, we confine the number of considered cases to a necessary minimum by considering only representatives of isomorphism classes.

In this scenario we are able to exploit additional information about the graphletisomorphisms to speed up the isomorphism checking. The checking procedure, however, is still computational expensive. Therefore we introduce the following means to reduce the number of required isomorphism checks.

Let $S$ be a set of cases. We decompose $S$ into several sets $S_{1}, S_{2}, \ldots$ For each graphlet $(G, v) \in S$ we use a serial version of Berkowitz' algorithm [1] to determine the coefficients of the characteristic polynomial of $G$ 's adjacency matrix. Graphlets are distributed into the sets $S_{i}$ according to the coefficients in their respective characteristic polynomial ${ }^{1}$.

Let $(G, v),\left(G^{\prime}, v^{\prime}\right)$ be graphlets. If they are isomorphic, then $G \cong G^{\prime}$ also holds. Therefore their adjacency matrices are permutations of each other. Thus they must have the same characteristic polynomial.

Altogether, two isomorphic graphlets will be contained in the same set $S_{i}$. Therefore it suffices to perform pairwise isomorphy checks on graphlets from the same set.

Also, in case the implementation of Berkowitz' algorithm was incorrect, we would not miss any relevant cases.

## 5 Completeness

Theorem 1. Let $S$ be the set of graphlets generated by our algorithm for an radius of 2 , a minimum degree of 3 and a maximum degree of 4 . Then for every relevant case $(G, v)$, relevant to algorithm, there is a case $\left(G^{\prime}, v^{\prime}\right) \in S$, such that $(G, v) \cong\left(G^{\prime}, v^{\prime}\right)$.

In this section we prove that an arbitrary graphlet with extent 2 is generated by our algorithm (for given <minDegree>,<maxDegree>). Recall the generation process' overview in Listing 1.1.

To improve the proof's readability, we will not distinct between isomorphic graphlets anymore. If $(G, v) \cong\left(G^{\prime}, v^{\prime}\right)$ we treat them as equal.

Proof. Let $(G, v)$ be a graphlet with extent $2, d(v)=4$ and $V(G)=\{v\} \cup O_{1} \cup O_{2}$ with $O_{1}=\left\{u_{1}, \ldots, u_{4}\right\}, O_{2}=\left\{w_{1}, \ldots, w_{n}\right\}$ where $n \leq 7$. Furthermore $d(x) \in$ $\{3,4\}$ for all $x \in V(G)$ and there is no $u_{i} \in O_{1}$ that has no neighbor in $O_{2}$. We will prove that $(G, v)$ is generated by our algorithm.

Let $T_{1}=\left(G\left[\{v\} \cup O_{1}\right], v\right)$ without edges in $O_{1}$. In Line 1 the call to generateStars generates only the 4 -star graphlet. Since $d(v)=4$ we know that $T_{1}$ is generated in the first line.

Consider Line 2 and assume that $T_{1}$ has been generated so far. Let $T_{2}=$ $\left(G\left[\{v\} \cup O_{1}\right], v\right)$ be the graphlet induced by the first orbit $O_{1}$ and the anchor vertex $v$. Since $(G, v)$ is a relevant case the edges in $E[G] \cap\binom{O_{1}}{2}$ are also added in one path of the exhaustive search tree employed by makeIntraOrbit1Edges. Therefore $T_{2}$ is generated by the second line.

Since, during the proof, we do not distinguish between isomorphic graphlets the pickRepresentatives-calls are not interesting.

Consider Line 5. Let, for some $u_{i} \in O_{1}, e\left(u_{i}\right)$ be the number of $u_{i}$ 's neighbors in $O_{2}$ w.r.t. $(G, v)$. Let $T_{3}=\left(G^{\prime}, v\right)$ where $V\left(G^{\prime}\right)=\{v\} \cup O_{1} \cup\left\{x_{1}, \ldots, x_{m}\right\}$

[^0]where $m=\sum_{i=1}^{4} e\left(u_{i}\right)$. Moreover $E\left(G^{\prime}\right)=\left\{\left\{v, u_{1}\right\}, \ldots,\left\{v, u_{4}\right\}\right\}$ and every $u_{i}$ is connected to $e\left(u_{i}\right)$ unique vertices in $\left\{x_{1}, \ldots, x_{m}\right\}$. Hence for all $x_{i}$ it holds $d\left(x_{i}\right)=1$. So $T_{3}$ equals $T_{2}$ with new vertices of degree 1 attached to $O_{1}$.

Since the call to appendTrees performs an exhaustive search, at least one of the leafs in the search tree provides $T_{3}$ (under the assumption that $T_{2}$ was obtained by the previous steps).

Consider Line 6 and assume $T_{3}$ was generated by now. Let $T_{4}=(G, v)$ but without anonymous edges and without edges in the second orbit. Since foldLeaves performs an exhaustive search on all possibilities to fold vertices, we only need to show that $T_{3}$ can be folded into $T_{4}$.

Let $x \in O_{2}\left(T_{4}\right)$ and $y_{1}, \ldots, y_{k}$ its neighbors in $O_{1}$. The $y_{i}$ have $e\left(y_{i}\right)$ neighbors with degree 1 . For each $y_{i}, y_{i+1}$ we take one of their unused neighbors $n_{i}, n_{i+1}$ in $O_{2}$ and fold them together. This is always possible since $N\left[n_{i}\right] \cap N\left[n_{i+1}\right]=$ $\left\{y_{i}\right\} \cap\left\{y_{i+1}\right\}=\emptyset$. We obtain a new vertex $z$ that is connected to $y_{i}, y_{i+1}$. We can now fold $z, y_{i+2}$, etc. Afterwards all $y_{i}$ have been folded into a single new vertex which resembles $x$ in $T_{4}$. We employ the same strategy for the remaining vertices in $O_{2}\left(T_{4}\right) \backslash\{x\}$. After we have done this, $T_{3}=T_{4}$. Moreover, the number of available vertices for folding is always sufficient, since the number of edges between $O_{1}$ and $O_{2}$ are not changed during folding.

Thus, under the assumption that $T_{3}$ is generated by the previous steps, we will obtain $T_{4}$ in Line 6 .

Let $T_{5}=(G, v)$ without any anonymous edges. By the same argument as regarding the second line, $T_{5}$ is generated under the assumption that $T_{4}$ was generated before.

In the last step, we perform an exhaustive search on the possibilities to add anonymous edges. Assuming that $T_{5}$ was generated by the previous steps, at least one leaf in the search tree will provide $(G, v)$.

Thus, neglecting isomorphisms, $(G, v)$ will be generated by the algorithm. Therefore the algorithm generates all relevant cases.

Since the completeness is crucial for the validity of Kneis, Langer, and Rossmanith's work [3], Reidl \& Sánchez Villaamil [5] devised a more readable - and therefore slower - program, used to verify that the presented algorithm generates all relevant cases. For information on their implementation refer to the respective technical report [5].

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