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Kyoto University
A Scheme for Generating Rooted Graphs with Reflectional Block Structures

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Abstract

In this paper, we consider an arbitrary class $\mathcal{H}$ of rooted graphs such that each biconnected component is given by a representation with reflectional symmetry, which allows a rooted graph to have several different representations, called embeddings. We give a general framework to design algorithms for generating embeddings of all graphs in $\mathcal{H}$ without repetition. The framework yields an efficient generation algorithm for a class $\mathcal{H}$ if the class $\mathcal{B}$ of biconnected graphs used in the graphs in $\mathcal{H}$ admits an efficient generation algorithm.

1 Introduction

Generation of restricted graphs or graphs with configurations has many applications in various fields such as machine learning and chemoinformatics. For example, Horváth et al. [3] reported that 94.3% of chemical compounds in NCI chemical database have outerplanar structures. Generation of trees and outerplanar graphs can be used for many purposes including the inference of structures of chemical compounds [5], virtual exploration of chemical universe [6], and reconstruction of molecular structures from their signatures [2]. Stereoisomers of chemical graphs can be treated as graphs with three-dimensional configurations, and recently an efficient generation algorithm for tree structured chemical graphs has been proposed [4].

The common idea behind most of the recent efficient generation algorithms (e.g., [8, 7, 9]) is to define a unique object for each of all objects as its “the parent,” which induces a rooted tree of all objects, called the family tree $\mathcal{F}$. Then all objects can be generated one by one according to the depth-first traversal of the family tree $\mathcal{F}$. For example, Nakano [7] presented an efficient algorithm that generates all triconnected rooted plane graphs in constant time per each, where a plane graph is one of the representations of a planar graph based on embeddings in the plane. Note that possibly two different plane graphs may be isomorphic to the same planar graph, if we ignore their embeddings.

Objects to be generated are often encoded into mathematically tractable representations. For example, a rooted unordered tree is represented by a rooted ordered tree by introducing a total order among the siblings of each vertex in the tree. Hence the representation of a rooted unordered tree has a symmetry around each vertex. In order to generate rooted unordered trees as rooted ordered trees without duplication, we choose one of all rooted ordered trees of a rooted unordered tree $T$ as the “canonical representation” of $T$. Then all canonical representations will be generated one by one according to the depth-first traversal of the family tree in such a way that a new one is generated by attaching a new leaf vertex to the immediately previous output and/or by deleting a few leaf vertices from the previous one (e.g., [9]). The algorithms output only a constant-size difference between two consecutive trees in the series of all canonical representations, achieving a constant time generation per each output.

Recently, based on the tree generation algorithm proposed by Nakano and Uno [8, 9], Fujiiwa et al. [1] and Ishida et al. [5] presented an efficient branch-and-bound algorithm for generating treelike chemical graphs, whose implementation is available as a web server*. Currently we aim to provide an

*http://sunflower.kuicr.kyoto-u.ac.jp/tools/enumol/
efficient branch-and-bound algorithm for generating chemical graphs for a wider class of graphs than trees such as outerplanar graphs in our web server.

In this paper, we propose a new method that enables us to treat the reflectional symmetry of biconnected components separately from that of the symmetry that arises from the tree-like combination of biconnected components in designing generation algorithms. For this, we consider an arbitrary class $\mathcal{H}$ of rooted graphs such that each biconnected component is given by a representation with reflectional symmetry, which allows a rooted graph to have several different representations, called “embeddings.” We give a general framework to design of algorithms for generating embeddings of all graphs in $\mathcal{H}$. The framework yields an efficient generation algorithm for a class $\mathcal{H}$ as long as an efficient generation algorithm for the class $\mathcal{B}$ of biconnected graphs used in graphs in $\mathcal{H}$ is available.

2 Preliminaries

For two sequences $A$ and $B$, let $A > B$ mean that $A$ is lexicographically larger than $B$, and let $A \geq B$ mean that $A > B$ or $A = B$. Let $A \sqsupset B$ mean that $B$ is a prefix of $A$ and $A \neq B$, and let $A \gg B$ mean that $A > B$ but $B$ is not a prefix of $A$. Let $A \supseteq B$ mean that $A \sqsupset B$ or $A = B$, i.e., $B$ is a prefix of $A$.

Throughout the paper, a graph stands for a simple undirected graph, which is denoted by a pair $H = (V, E)$ of a vertex set $V$ and an edge set $E$. A graph is treated as a labeled graph in which all vertices receive distinct vertex names unless stated otherwise. The set of vertices and the set of edges of a given graph $H$ are denoted by $V(H)$ and $E(H)$, respectively.

A graph with a vertex $r$ designated as the root is called a rooted graph or a graph rooted at $r$. For each biconnected component $B$ of a graph rooted at a vertex $r$, the root $r(B)$ of $B$ is defined to be the unique vertex $v \in V(B)$ closest to $r$, and treat $B$ as a graph rooted at $r(B)$. Let $V'(B)$ denote $V(B) - \{r(B)\}$. For a vertex $v$, let $B(v)$ denote the biconnected component with $v \in V'(B)$ if any. The depth $d(B)$ of a biconnected component $B$ is defined by the number of biconnected components which edge sets intersect with a simple path from a vertex in $V'(B)$ to the root $r$.

Two rooted graphs $H_1$ and $H_2$ are rooted-isomorphic if they admits an isomorphic bijection by which the roots of $H_1$ and $H_2$ correspond each other. Such a bijection is called rooted-isomorphic.

In this paper, we define a block to be a rooted biconnected graph with a configuration such as an embedding into the plane. Two blocks are called equivalent if the biconnected graphs of these blocks admit a rooted-isomorphic bijection under the configuration, where these biconnected graphs may be a rooted-isomorphic bijection which does not obey the configuration. We assume that, for each block $B$, either (i) no other block $B'$ is equivalent to $B$ under the configuration, where $B$ is called asymmetric or (ii) there is exactly one distinct block $B'$ which is equivalent to $B$, and $B$ and $B'$ admit a symmetry of order 2 which is given by an automorphism $\psi$ such that $V_1(B) = \{\psi(v) \mid v \in V_2(B)\}$ and $\psi(v) = v$, $v \in V_3(B)$ for a partition $V_1(B)$, $V_2(B)$ and $V_3(B)$ of the vertex set $V(B)$. A block $B$ in (ii) is called symmetric. A level $\ell$ of vertices in a block $B$ is an assignment of a positive integer $\ell(v)$ for each vertex in $V'(B)$ if it satisfies the following property: (1) For an asymmetric block $B$, it holds $\ell(v) \neq \ell(u)$ for every two distinct vertices $u, v \in V'(B)$; and (2) For a symmetric block $B$, there is a partition $V_1(B)$, $V_2(B)$ and $V_3(B)$ of $V(B)$ such that the vertices in each $V_i$ receive distinct integers and $\ell(v) = \ell(\psi(v))$ for all $v \in V_i(B)$.

Let $\mathcal{B}$ denote a set of such blocks. More formally, we assume that a parent-child graph relationship $(P_\mathcal{B}, C_\mathcal{B})$ is defined over all blocks in $\mathcal{B}$: A block $B$ is called the seed block if it has no parent in $\mathcal{B}$. For each non-seed block $B$, $P_\mathcal{B}(B')$ denotes a block $B' \in \mathcal{B}$ that is defined as the parent of $B$, and $C_\mathcal{B}(B')$ denotes the set of children of $B'$, i.e., blocks $B''$ with $B' = P_\mathcal{B}(B'')$. Also assume that there exists signature $\gamma$ of all blocks in $\mathcal{B}$ such that (S1) every two blocks $B$ and $B'$ are equivalent under the configuration of $\mathcal{B}$ if and only if $\gamma(B) = \gamma(B')$; (S2) there is a parent-child relationship among blocks in $\mathcal{B}$ such that no child of a block has less number of vertices than its parent has; and (S3) $\mathcal{B}$ contains exactly one seed block $\tilde{B}$. Moreover, $\gamma$ is called monotone with respect to the number of vertices if the followings hold: (S4) for any
two blocks $B', B'' \in C_{B}(B), B \in \mathcal{B}$, if $|V(B')| > |V(B'')|$ then $\gamma(B') > \gamma(B'')$; and (S5) for any block $B \in \mathcal{B}$, $\gamma(B') > \gamma(B)$ holds for all children $B' \in C_{B}(B)$, and $|V(B')| > |V(B)|$, for all $B' \in C_{B}(B)$.

We consider the set $\mathcal{H}$ of such rooted graphs in which each biconnected component is represented by a block $B \in \mathcal{B}$. In a rooted graph $H \in \mathcal{H}$, a block $B$ with $r(B) = v$ is called the child-block of $v$. For two blocks $B$ and $B'$ with $r(B') \in V'(B)$ in a rooted graph $H \in \mathcal{H}$, we say that $B$ is the parent-block of $B'$ and that $B'$ is a child-block of $B$. For two blocks $B$ and $B'$ such that $r(B')$ appears in any path from $r(B)$ to $r_{G}$, we call $B'$ an ancestor-block of $B$ and $B$ an descendant-block of $B'$, where $B$ is an ancestor-block and a descendant-block of itself. Two blocks $B$ and $B'$ are called incomparable if $B$ is neither an ancestor-block of $B'$ nor a descendant-block of $B'$. Given two incomparable blocks $B_{1}$ and $B_{2}$, we define the least common ancestor $lca(B_{1}, B_{2})$ of $B_{1}$ and $B_{2}$ to be either the common ancestor-block $B_{3}$ of $B_{1}$ and $B_{2}$ such that $B_{1}$ and $B_{2}$ are descendant-block of different child-blocks of $B_{3}$, or the common root $r(B_{1}') = r(B_{2}')$ of ancestor-blocks $B_{i}'$ of $B_{i}$, $i = 1, 2$ with $B_{1}' \neq B_{2}'$. If $B_{1} = B_{2}$, then define $lca(B_{1}, B_{2})$ to be block $B_{1}$. If $B_{1} \neq B_{2}$ and $B_{1}$ is an ancestor-block of $B_{2}$, then $lca(B_{1}, B_{2})$ is defined to be the root $r(B_{3}) \in V'(B_{1})$ of the child-block $B_{3}$ of $B_{1}$ such that $B_{3}$ is an ancestor-block of $B_{2}$.

![Figure 1: (a), (b) Two left/right-assignments of $V^{R}(B)$ and $V^{L}(B)$ to $V_{2}(B)$ and $V_{3}(B)$ of a symmetric block $B$; (c) Spine $B^{1}, B^{2}, \ldots, B^{p}$ of an embedding $G$.](image)

In this paper, we consider a class $\mathcal{H}$ of all embeddings over a class $\mathcal{B}$ of blocks; For each block $B$, we define left/right-assignments $V^{c}(B), V^{l}(B)$ and $V^{r}(B)$ as follows. For the vertex set $V_{1}(B)$, we always set $V^{c}(B) = V_{2}(B)$. For the vertex sets $V_{1}(B)$ and $V_{2}(B)$, there are two choices, either $V^{l}(B) = V_{1}(B), V^{r}(B) = V_{2}(B)$ or $V^{l}(B) = V_{2}(B), V^{r}(B) = V_{1}(B)$, as shown in Fig. 1(a) and (b). For an asymmetric block $B \in \mathcal{B}$, let $V^{c}(B) = V(B)$ and $V^{l}(B) = V^{r}(B) = \emptyset$. For each vertex $v \in V(B)$, define the side side(v) of $v$ in $B$ to be the index $i$ such that $v \in V_{i}(B)$. For convenience, we call a vertex in $V^{r}(B)$ (resp., $V^{l}(B)$ and $V^{c}(B)$) left (resp., right and central). We assume that $V^{c}(B)$, $V^{l}(B)$ and $V^{r}(B)$ denote subsets of these vertices to which other blocks are allowed to append.

We define the depth $\delta(v)$ of a vertex $v$ in a rooted graph $H \in \mathcal{H}$ to be $\delta(v) = (d(B), \ell(v))$ for the block $B$ of $H$ with $v \in V'(B)$ and the level $\ell(v)$ of $v$ in $B$. We say that two rooted graphs $H_{1}, H_{2} \in \mathcal{H}$ are depth-isomorphic if and only if they admit a rooted-isomorphic bijection $\phi$ that maps each vertex $v \in V(H_{1})$ to a vertex $\phi(v) \in V(H_{2})$ with $\delta(\phi(v)) = \delta(v)$.

We define an embedding of a rooted graph $H \in \mathcal{H}$ as follows. For each vertex $v$, let $BS[v]$ denote a sequence $(B_{1}, B_{2}, \ldots, B_{k})$ of all child-blocks of $v$ such that $B_{1}, B_{2}, \ldots, B_{k}$ appear in this order, where we say that $B_{1}, B_{2}, \ldots, B_{k}$ appear from left to right. For a symmetric block $B$ in an embedding $G$, there
are two left/right-assignments. An embedding of a rooted graph $H \in \mathcal{H}$ is specified by sequences $BS[v]$ of cut-vertices in $H$ and left/right-assignments of all symmetric blocks $B$. A rooted graph $H \in \mathcal{H}$ may have several different embeddings. Two embeddings $G_1$ and $G_2$ of $H_1, H_2 \in \mathcal{H}$ are equivalent if $H_1$ and $H_2$ are depth-isomorphic, i.e., $G_1$ can be obtained from $G_2$ by changing the orderings of blocks in $BS[v]$ for some vertices $v$ and exchanging the left/right-assignments of some symmetric blocks.

## 3 Signature of Embeddings

In this section, we define signature $\sigma$ of embeddings of graphs in $\mathcal{H}$. For an embedding $G$ of a graph $H \in \mathcal{H}$, let $r_G$ denote the root of $H$. For a block $B$, let $V_{cut}(B)$ denote the set of cut-vertices of $v \in V'(B)$.

Let $V_{cut}^L(B) = V_{cut}(B) \cap V^L(B)$. Similarly for $V_{cut}^R(B)$ and $V_{cut}^c(B)$. For a block $B$, a child-block $B'$ of $B$ is called a left (resp., right and central) child-block if $r(B') \in V^L(B)$ (resp., $r(B') \in V^R(B)$ and $r(B') \in V^c(B)$), where $V^L(B) = V^R(B) = \emptyset$. In particular, a left (resp., right and central) child-block $B_i$ of $B$ is called the first left (resp., right and central) child-block if $B$ has no other left (resp., right and central) child-block $B_j$ with $j < i$.

We define the key $key(v)$ of a vertex $v \in V(B)$ of a block $B$ in an embedding $G$ to be $key(v) = (side(v), \ell(v))$ and define a total order among keys by the lexicographical order with the first entry side and the second entry $\ell$.

We define the tip $t(B)$ of a block $B$ with $V_{cut}(B) \neq \emptyset$ in an embedding $G$ to be the vertex $v \in V_{cut}(B)$ with the smallest key. In other words, tip $t(B)$ is chosen as follows:

1. $V_{cut}^L(B) \neq \emptyset$: Define $t(B)$ to be the right vertex $v \in V_{cut}^R(B)$ with the smallest $\ell(v)$;
2. $V_{cut}^R(B) = \emptyset$ and $V_{cut}^c(B) \neq \emptyset$: Define $t(B)$ to be the left vertex $v \in V_{cut}^L(B)$ with the smallest $\ell(v)$; and
3. $V_{cut}^L(B) = V_{cut}^R(B) = \emptyset$, and $V_{cut}^c(B) \neq \emptyset$: Define $t(B)$ to be the central vertex $v \in V_{cut}^c(B)$ with the smallest $\ell(v)$.

For a block $B$ such that $V_{cut}(B) \neq \emptyset$, the successor of $B$ is defined to be the rightmost block in $BS[t(B)]$. The spine $\sigma(G)$ of $G$ is defined to be the sequence of all successors starting from the rightmost block $B^1 \in BS[r_G]$ by $B^1, B^2, \ldots, B^p$, where $B^1$ is the rightmost block in $BS[r_G]$, and each $B^i (i \geq 2)$ is the successor of $B^{i-1}$. See Fig. 1(c). The last block $B^p$ is called the tip-block of $G$.

The parent-embedding $\mathcal{P}_H(G)$ of an embedding $G$ is defined as follows.

1. If the tip-block $B$ of $G$ is not a block equivalent to the seed block $\tilde{B}$ then $\mathcal{P}_H(G)$ is defined to be the embedding obtained by replacing $B$ with its parent $\mathcal{P}_B(B)$.

2. Otherwise, $\mathcal{P}_H(G)$ is defined to be the embedding obtained by removing the vertices in $V'(B)$ from $G$.

We introduce a total order $\pi(G)$ among all blocks in an embedding $G$ as follows. Let $G$ have $K$ blocks, let $\mathcal{P}_H(G), i = 0, 1, \ldots, K - 1$ denote the embedding $\mathcal{P}_H(\mathcal{P}_H^{i-1}(G))$. Let $\pi(G) = (B_1, B_2, \ldots, B_K)$, where $B_i$ is the tip-block of $\mathcal{P}_H^{i-1}(G)$, i.e., the tip-block of the embedding obtained after repeating removal of the tip-block $K - i$ times.

The code $\gamma'(B)$ of a block $B$ in $G$ is defined to be

$$\gamma'(B) = (d(B), side(r(B)), \ell(r(B)), \gamma(B)),$$

where $side(r(B))$ and $\ell(r(B))$ are the side and level of a vertex $v$ in the block $B(v)$ and we set $side(r(B)) = \ell(r(B)) = 0$ if $r(B) = r_G$. The signature $\sigma(G)$ of an embedding $G$ is defined to be

$$\sigma(G) = [\gamma'(B_1), \gamma'(B_2), \ldots, \gamma'(B_K)]$$

for the order $\pi(G) = (B_1, B_2, \ldots, B_K)$ of all blocks in $G$. Observe that

$$\sigma(\mathcal{P}_H(G)) = \begin{cases} [\gamma'(B_1), \gamma'(B_2), \ldots, \gamma'(B_{K-1})] & \text{if } B_K \text{ equivalent to } \tilde{B} \\ [\gamma'(B_1), \gamma'(B_2), \ldots, \gamma'(B_{K-1}), \gamma'(\mathcal{P}_B(B_K))] & \text{otherwise,} \end{cases}$$
where $\delta(r(\mathcal{P}(B_K))) = \delta(r(B_K))$.

For two indices $i$ and $j$ ($i \leq j$), let $\sigma_{i,j}(G)$ denote the subsequence
$$\sigma_{i,j}(G) = [\gamma(B_i), \gamma(B_{i+1}), \ldots, \gamma(B_j)]$$
for the blocks $B_i, B_{i+1}, \ldots, B_j$ which appear consecutively in $\pi(G)$. Let $G(B)$ denote the embedding induced from $G$ by $B$ and all descendant-blocks of $B$. For a block $B$, $G(B)$ consists of some blocks $B_1, B_{i+1}, \ldots, B_j$ that appear in this order in $\pi(G)$, and let $\sigma(G(B); G)$ denote $\sigma_{i,j}(G)$. Then signature $\sigma$ has the following property.

**Lemma 1** Let $G$ and $G'$ be two embeddings of a rooted graph $H \in \mathcal{H}$. Then $G$ and $G'$ are the same embedding if and only if $\sigma(G) = \sigma(G')$.

**Proof.** Since $\sigma(G)$ of an embedding $G$ is uniquely determined by definition, we see that $G$ and $G'$ are the same embedding only if $\sigma(G) = \sigma(G')$.

We show that, for any embedding $G$, no other embedding $G'$ satisfies $\sigma(G') = \sigma(G)$. Let $\pi(G) = (B_1, B_2, \ldots, B_K)$, and let $G_1$ denote the embedding induced from $G$ by the first $i$ blocks in $\pi(G)$, i.e., $G_1$ is obtained from $G$ by removing blocks $B_{i+1}, B_{i+2}, \ldots, B_K$. Let $\sigma_i = [\gamma(B_1), \gamma(B_2), \ldots, \gamma(B_i)]$, $i = 1, 2, \ldots, K$. For $i = 1$, we see that only $G_1 = B_1$ can satisfy $\sigma(G_1) = \sigma_1$. Assuming that, for $i = j < K$, only embedding $G_j$ can satisfy $\sigma(G_j) = \sigma_j$, we show that only $G_{j+1}$ can admit signature $\sigma(G_{j+1}) = \sigma_{j+1}$. For any embedding $G''$ such that $\sigma(G'') = \sigma_{j+1}$, the last code $\gamma(B_{j+1}) = (d(B_{j+1}), \mathrm{side}(r(B_{j+1})), \ell(r(B_{j+1})), \gamma(B_{j+1}))$ in $\sigma_{j+1}$ specifies the tip-block of $G''$, and the embedding $G'''$ obtained from $G''$ by removing the tip-block $B_{j+1}$ satisfies $\sigma(G''') = \sigma_j$. By the induction hypothesis, $G'''$ is $G_j$. Note that $G''$ is obtained from $G_j$ by attaching $B_{j+1}$. It is sufficient to show that a way of attaching $B_{j+1}$ to $G_j$ is uniquely determined by the information in $\gamma'(B_{j+1})$. Code $\gamma'(B_{j+1})$ specifies the depth of a block $B$ in $G_j$ to which block $B_{j+1}$ is attached. There may be more than one such block $B$, but exactly one such block $B$ is determined as the one in the spine of $G_j$, since $B_{j+1}$ cannot be the tip-block of the resulting embedding if $B_{j+1}$ is attached to any other block than those in the spine of $G_j$. The vertex to which $B_{j+1}$ is allowed to attach is also uniquely determined by $\mathrm{side}(r(B_{j+1}))$ and $\ell(r(B_{j+1}))$, since vertices in each of $V_1(B)$, $V_2(B)$, and $V_3(B)$ are assigned with distinct levels $\ell$. This shows that only $G_{j+1}$ satisfies $\sigma(G_{j+1}) = \sigma_{j+1}$, as required.

4 Canonical Embeddings

For each block $B \in BS[v]$, $G(B)$ consists of blocks $B = B_1, B_{i+1}, \ldots, B_j$ which appear consecutively in $\pi(G)$, and we denote by $\sigma(G(B); G)$ the subsequence
$$\sigma_{i,j}(G) = [\gamma(B_i), \gamma'(B_{i+1}), \ldots, \gamma'(B_j)].$$

An embedding $G$ is called left-sibling-heavy at a block $B \in BS[v] = (B_1', B_2', \ldots, B_p')$ if $B = B_1'$ or $\sigma(G) \geq \sigma(G')$ holds for the embedding $G'$ obtained from $G$ by exchanging the order of $B_{i-1}'$ and $B_i'$ in $BS[v]$.

**Lemma 2** An embedding $G$ is left-sibling-heavy at a block $B_i' \in BS[v] = (B_1', B_2', \ldots, B_p')$ with $i \geq 2$ if and only if $\sigma(G(B_{i-1}')); G) \geq \sigma(G(B_i'); G)$ holds.

**Proof.** Let $G'$ be the embedding obtained from $G$ by exchanging the order of $B_{i-1}'$ and $B_i'$ in $BS[v]$. Signatures $\sigma(G)$ and $\sigma(G')$ have a common subsequence before the subsequences $[\sigma(G(B_{i-1}')); G), \sigma(G(B_i'); G)]$ and $[\sigma(G(B_i')); G'), \sigma(G(B_{i-1}')); G')$, respectively.
Note that $\sigma(G(B');G') = \sigma(G(B');G)$ and $\sigma(G(B_{-1}');G') = \sigma(G(B_{-1}');G)$. Hence $\sigma(G) \geq \sigma(G')$ holds if and only if

$$[\sigma(G(B_{-1}');G), \sigma(G(B');G)] \geq [\sigma(G(B');G), \sigma(G(B_{-1}');G)].$$

Since the lemma holds when $\sigma(G(B_{-1}');G) = \sigma(G(B');G)$, it suffices to show that $\sigma(G(B_{-1}');G) > \sigma(G(B');G)$ implies

$$[\sigma(G(B_{-1}');G), \sigma(G(B');G)] > [\sigma(G(B');G), \sigma(G(B_{-1}');G)],$$

and that $\sigma(G(B');G) > \sigma(G(B_{-1}');G)$ implies

$$[\sigma(G(B_{-1}');G), \sigma(G(B');G)] > [\sigma(G(B');G), \sigma(G(B_{-1}');G)].$$

By symmetry, it is sufficient to show the former.

Assume that $\sigma(G(B_{-1}');G) > \sigma(G(B');G)$. If $\sigma(G(B_{-1}');G) \geq \sigma(G(B_{-1}');G)$ holds, then we have $[\sigma(G(B_{-1}');G), \sigma(G(B');G)] > [\sigma(B');G'), \sigma(G(B_{-1}');G')$]. Then we consider the case where $\sigma(G(B_{-1}');G) \geq \sigma(G(B');G)$ or $[\sigma(G(B_{-1}');G), \sigma(G(B');G)] > [\sigma(G(B_{-1}');G), \sigma(G(B');G)]$. In this case, the first code $\gamma(B_{a})$ in $\sigma(G(B_{-1}');G)$ is compared with the $(\sigma(G(B_{-1}');G) + 1)$st code $\gamma(B_{a})$ in $\sigma(G(B_{-1}';G))$.

Let $B_{a}$ (resp., $B'_{a}$) be the block such that $r(B_{a}) \in V'(B_{a})$ (resp., $r(B'_{a}) \in V'(B'_{a})$). Then the first entry in $\delta(r(B_{a}))$ of $\gamma'(B_{a})$ is $d(B_{a}') = d(B_{-1}') - 1$, whereas the first entry $d(B_{a}')$ in $\delta(r(B'_{a}))$ of $\gamma'(B'_{a})$ satisfies $d(B_{a}') \geq d(B_{-1}')$. Hence $\gamma'(B_{a}) > \gamma'(B'_{a})$ holds, as required.

For a symmetric block $B$ in an embedding $G$, let $G/B'$ denote the flipped embedding of $G$ that is obtained by exchanging the vertex set $V(B)$ with $V'(B)$; i.e., re-attach all child-blocks $B'$ at each vertex $u \in V(B)$ (resp., $u \in V'(B)$) to the vertex $u' \in V'(B)$ (resp., $u' \in V(B)$) with $\delta(u') = \delta(u)$.

An embedding $G$ is called left-side-heavy at a symmetric block $B \in BS[v]$ if $\sigma(G) \geq \sigma(G')$ holds for the embedding $G' = G/B'$ obtained from $G$ by flipping $B$.

For a block $B$, let $B = B_{1}, B_{1}+1, \ldots, B_{j}$ be the blocks in $G(B)$ that appear in this order in $\pi(G)$. Sequence $\sigma(G(B);G)$ consists of four subsequences: the first one is $\sigma_{1}(G) = [\delta(r(B)), \gamma(B)]$, the second $\sigma_{t_{1}+1,i_{c}}(G)$, the second $\sigma_{t_{i_{c}}+1,i_{L}}(G)$, and the second $\sigma_{t_{L}+1,j}(G)$, $B_{k}$ with $i + 1 \leq k \leq i_{c}$ (resp., $i_{c} + 1 \leq k \leq i_{L}$ and $i_{L} + 1 \leq k \leq j$) is a descendant-block of a vertex $u \in V_{cut}^{i}$ (resp., $u \in V_{cut}^{i}$ and $u \neq V_{cut}^{i}$). We denote these subsequences by $\sigma(B;G)$, $\sigma_{c}(G(B);G)$, $\sigma_{L}(G(B);G)$, and $\sigma_{C}(G(B);G)$, respectively. Hence

$$\sigma(G(B);G) = [\sigma(B;G), \sigma_{c}(G(B);G), \sigma_{L}(G(B);G), \sigma_{C}(G(B);G)].$$

We define the flipped code $\overline{\gamma}(B)$ of $\gamma(B)$ to be the code obtained from $\gamma(B)$ by replacing the value of the second entry side $1$ (resp., side $0$) with side $0$ (resp., side $1$). Let $\overline{\gamma}(B;G)$ (resp., $\overline{\gamma}_{c}(G(B);G)$) denote the sequence obtained from $\sigma_{c}(G(B);G)$ (resp., $\sigma_{C}(G(B);G)$) by replacing $\gamma'(B')$ with $\overline{\gamma}'(B')$ for all blocks $B'$ such that $r(B') \in V'(B)$. Denote $\overline{\gamma}(B;G) = [\sigma(B;G), \sigma_{c}(G(B);G), \sigma_{L}(G(B);G), \sigma_{C}(G(B);G)]$.

**Lemma 3** An embedding $G$ is left-side-heavy at a symmetric block $B \in BS[v]$ if and only if it holds $\sigma_{L}(G(B);G) \geq \overline{\sigma}_{L}(G(B);G)$.

**Proof.** Let $G' = G/B'$. Signatures $\sigma(G)$ and $\sigma(G')$ have a common subsequence before their subsequences $[\sigma_{c}(G(B);G), \sigma_{L}(G(B);G)]$ and $[\sigma_{L}(G(B);G), \sigma_{C}(G(B);G)]$ start, respectively. Note that $\sigma(G')$ is obtained from $\sigma(G)$ by replacing $\sigma_{L}(G;B;G)$ with $\sigma_{L}(G;B;G)$. Hence

$$\sigma(G) \geq \sigma(G') \Leftrightarrow [\sigma_{L}(G(B);G), \sigma_{C}(G(B);G)] \geq [\overline{\sigma}_{L}(G(B);G), \overline{\sigma}_{C}(G(B);G)].$$

For simplicity, let $\sigma^{*}$ denote $\sigma^{*}(G(B);G)$. Similarly for $\sigma_{L}$.

Since (2) holds when $\sigma_{L} = \sigma_{L}$, it suffices to show that $\sigma_{L} > \overline{\sigma}_{L}$ (resp., $\overline{\sigma}_{L} > \overline{\sigma}_{L}$) implies

$$[\sigma_{L}, \sigma_{L}] > [\overline{\sigma}_{L}, \overline{\sigma}_{L}]$$
(resp., $|\overline{\sigma_{L}}| > |\sigma_{R}|$). We prove the former (the latter can be treated symmetrically).

Assume $|\sigma_{L}| > |\overline{\sigma_{R}}|$. If $|\sigma_{L}| > |\overline{\sigma_{R}}|$ then we have $|\sigma_{L}| > |\overline{\sigma_{R}}|$. We assume $|\sigma_{L}| > |\overline{\sigma_{R}}|$ holds. If $|\sigma_{L}| = |\overline{\sigma_{R}}|$, then we again obtain $|\sigma_{L}| > |\overline{\sigma_{R}}|$. Assume that $|\sigma_{L}| > |\overline{\sigma_{R}}|$ holds. In this case, the first code $\gamma'(B_{a})$ in $\overline{\sigma_{R}}$ is compared with the $(|\sigma_{L}| + 1)$st code $\gamma'(B_{a})$ in $\sigma_{L}$, and it suffices to show that $\gamma'(B_{a}) > \gamma'(B_{a})$. Let $B'_{a}$ be the block such that $r(B_{a}) \in V'(B'_{a})$ (resp., $r(B_{a}) \in V'(B'_{a})$), and let $\gamma'(B_{a}) = (d(B_{a}), \ell(r(B_{a})), \gamma'(B_{a}))$ and $\gamma'(B_{a}) = (d(B_{a}), \ell(r(B_{a})), \gamma(B_{a}))$. It holds $d(B'_{a}) = d(B_{a}) + 1 = d(B_{a})$. If $d(B'_{a}) = d(B_{a}) + 1$ holds, then we have $\gamma'(B_{a}) = \gamma'(B_{a})$ by $r(B_{a}) = 2 > 1 = \ell(r(B_{a}))$, as required.

An embedding $G$ is called canonical if it is left-sibling-heavy and left-side-heavy at all symmetric blocks in $G$.

**Lemma 4** Let $G$ be an embedding of a rooted graph $H \in \mathcal{H}$. Then $G$ is canonical if and only if $\sigma(G)$ is lexicographically maximum among all $\sigma(G')$ of embeddings $G'$ of $H$.

**Proof.** (i) Only if part: Let $G$ be an embedding of a rooted graph $H \in \mathcal{H}$ such that $\sigma(G)$ is lexicographically maximum. To derive a contradiction, assume that $G$ is not canonical.

If $G$ is not left-sibling-heavy at some block $B_{i} \in BS[v] = (B'_{1}, B'_{2}, \ldots, B'_{k})$, then $\sigma(G(B'_{i}) ; G) > \sigma(G(B_{i-1}) ; G)$ holds by Lemma 2. Hence by the definition of left-sibling-heaviness, the embedding $G'$ obtained from $G$ by exchanging the order of $B'_{i-1}$ and $B'_{i}$ in $BS[v]$ has signature $\sigma(G')$ which is lexicographically larger than $G$.

If $G$ is not left-side-heavy at some symmetric block $B_{i}$, then it holds $\overline{\sigma(G(B'_{i}))} > \sigma(G(B_{i}) ; G)$ by Lemma 3. Hence by the definition of left-side-heaviness, the embedding $G' = G/B'_{i}$ obtained from $G$ by flipping $B_{i}$ has signature $\sigma(G')$ which is lexicographically larger than $\sigma(G)$.

(ii) If part: By (i), any embedding $G'$ is canonical if $\sigma(G')$ is lexicographically maximum. Hence it suffices to show that a canonical embedding is unique. Let $v$ be a cut-vertex with the largest depth in $G$. The ordering of blocks $B'_{1}, B'_{2}, \ldots, B'_{k} \in BS[v]$ in $G$ lexicographically maximizes $|\gamma'(B'_{1}), \gamma'(B'_{2}), \ldots, \gamma'(B'_{k})|$, and is unique, since either $\gamma'(B'_{i}) > \gamma'(B'_{i})$ or $\gamma'(B'_{i}) > \gamma'(B'_{i})$ whenever blocks $B'_{i}$ and $B'_{i}$ are distinct. Also let $B$ be a symmetric block with the largest depth. Then $\sigma(G(B) ; G)$ takes the lexicographically maximum of $\sigma(G(B) ; G)$ and $\overline{\sigma(G(B) ; G)}$. By applying the argument in a bottom-up manner along $G$, we see that a canonical embedding is rooted-isomorphically unique.

**Lemma 5** For a canonical embedding $G$, its parent-embedding $\mathcal{P}_{H}(G)$ (if any) is a canonical embedding.

**Proof.** Let $G$ be a canonical embedding of a graph $H \in \mathcal{H}$. Hence $G$ satisfies all the inequalities in Lemmas 2 and 3. Let $B'_{1}, B'_{2}, \ldots, B'_{k}$ be the spine of $G$, let $G' = \mathcal{P}_{H}(G)$, and $H' \in \mathcal{H}$ be the graph represented by $G'$. Then $\sigma(G)$ is obtained from $\sigma(G)$ by deleting the last code $\gamma'(B'_{k})$ or replacing $\gamma'(B'_{k}) = (d(B'_{k}), \ell(r(B'_{k})), \gamma'(B'_{k}))$ with $(d(B'_{k}), \ell(r(B'_{k})), \gamma'(B'_{k}))$. In this case, all the inequalities in Lemmas 2 and 3 remain valid since such a change in the signature can make the right hand side of any of these inequalities smaller. Thus, $G'$ is also a canonical embedding of $H'$. 

Let $G$ be an embedding with $\sigma(G) = [\gamma'(B_{1}), \gamma'(B_{2}), \ldots, \gamma'(B_{K})]$, where $B_{K}$ is the tip-block of $G$. Let $v$ be a vertex in $G$. For a block $B_{i}$ which has an ancestor-block $B_{i}$ of $B_{i}$ with $v = r(B_{i})$, we call each block $B_{j}$ with $k \leq j \leq i$ a pre-block of $B_{i}$ to $v$, and define the pre-sequence $ps(v, B_{i})$ of $B_{i}$ to $v$ to be $\sigma_{k,i-1}(G) = [\gamma'(B_{k}), \gamma'(B_{k+1}), \ldots, \gamma'(B_{i-1})]$, where $ps(B_{i}, B_{i}) = \emptyset$ if $k = i$.

Let $B_{i}$ be a block in $G$. For a block $B_{i}$ which is a descendant-block of a left (resp., right/central) child-block of $B_{i}$, we define the initial ancestor-block $B_{i}$ of $B_{i}$ to $B_{i}$ to be the first left (resp., right/central) child-block of $B_{i}$, and call each block $B_{j}$ with $i' \leq j \leq i$ a pre-block of $B_{i}$ to $B_{i}$. Define the pre-sequence $ps(B_{i}, B_{i})$ of $B_{i}$ to $B_{i}$ to be $\sigma_{k,i-1}(G) = [\gamma'(B_{i}), \gamma'(B_{i+1}), \ldots, \gamma'(B_{i-k})]$.

A left (resp., right) child-block $B_{i}$ of a block $B$ is called opposing with a right (resp., left) child-block $B_{i}$ of $B$. Let $\gamma'(B) \simeq \gamma'(B')$ mean $\gamma'(B) = \gamma'(B')$ if block $B$ is opposing with $B'$, and $\gamma'(B) = \gamma'(B')$
Figure 2: Two possible cases where a block $B_j$ is pre-identical to a block $B_i$, (a) $\text{lca}(B_i, B_j)$ is a vertex $v$; (b) $\text{lca}(B_i, B_j)$ is a block $B_h$.

otherwise. For two subsequence $\sigma_{j,k}(G)$ and $\sigma_{j',k'}(G)$, let $\sigma_{j,k}(G) \simeq \sigma_{j',k'}(G)$ imply that $k' - j' = k - j \geq 0$ and $\gamma'(B_{j+i}) \simeq \gamma'(B_{j'+i})$, $i = 0, 1, \ldots, k - j$.

For a block $B_i$, a block $B_j$ with $j < i$ incomparable $B_i$ is called pre-identical to $B_i$ if one of the following conditions holds:

(i) $\text{lca}(B_i, B_j)$ is a vertex $v$, $\text{ps}(v, B_j) = \text{ps}(v, B_i)$, and the first pre-blocks of $B_i$ and $B_j$ to $v$ are immediately adjacent siblings at $v$. See Fig. 2(a).

(ii) $\text{lca}(B_i, B_j)$ is a block $B_h$ and $\text{ps}(B_h, B_j) \simeq \text{ps}(B_h, B_i)$. See Fig. 2(b).

Note that $\text{ps}(B_h, B_j) \simeq \text{ps}(B_h, B_i)$ holds only when $B_h$ is symmetric and the initial ancestor-block $B_x$ of $B_i$ (resp., $B_y$ of $B_j$) to $B_h$ is a right (resp., left) child-block of $B_h$. Hence conditions (i) and (ii) can be expressed by $\text{ps}(\text{lca}(B_i, B_j), B_j) \simeq \text{ps}(\text{lca}(B_i, B_j), B_i)$.

If $B_i$ has a left sibling $B_j$ at $v = r(B_i)$, then $B_j$ is pre-identical to $B_i$, where $\text{ps}(v, B_j) = \text{ps}(v, B_j) = \emptyset$. In a canonical embedding $G$, the first right child-block $B$ of a block $B_h$ has an opposing block such as the first left child-block $B_j$, since otherwise $G$ is not left-side-heavy. Hence $B_j$ is pre-identical to such block $B_i$.

**Lemma 6** For a block $B_d$ in a canonical embedding $G$, let $B_c$ and $B_b$ ($b < c < d$) be two blocks pre-identical to $B_d$. Then $\gamma'(B_c) \geq \gamma'(B_b) \geq \gamma'(B_d)$ holds. In particular, $\gamma'(B_d) \simeq \gamma'(B_c)$ implies $\gamma'(B_d) \simeq \gamma'(B_b)$.

**Proof.** Since $B_b$ is pre-identical to $B_i$, we have $\text{ps}(\text{lca}(B_d, B_b), B_b) \simeq \text{ps}(\text{lca}(B_d, B_b), B_b)$. This implies that there is a block $B_a$, $a < b$ pre-identical to $B_c$ and $\gamma'(B_a) \simeq \gamma'(B_c)$ holds. See Fig. 3. Since $B_c$ is pre-identical to $B_d$, we have $\text{ps}(\text{lca}(B_d, B_c), B_d) \simeq \text{ps}(\text{lca}(B_d, B_c), B_c)$. Hence $B_a$ is pre-identical to $B_b$. Since $G$ is canonical, it must hold $\gamma'(B_a) \geq \gamma'(B_b)$ and $\gamma'(B_b) \geq \gamma'(B_d)$. Hence it holds $\gamma'(B_c) = \gamma'(B_a) \geq \gamma'(B_b) \geq \gamma'(B_d)$, as required. Hence, $\gamma'(B_d) \simeq \gamma'(B_c)$ implies $\gamma'(B_b) \simeq \gamma'(B_d)$.

### 5 Generation Algorithm for Class $\mathcal{H}$

An embedding $G'$ is called a child-embedding of an embedding $G$ if $G = \mathcal{P}_{\mathcal{H}}(G')$. Let $\mathcal{C}_{\mathcal{H}}(G)$ denote the set of all canonical child-embeddings of an canonical embedding $G$. We define a family tree $\mathcal{F}_{\mathcal{H}}$ in which each canonical embedding $G$ is joined to its parent $\mathcal{P}_{\mathcal{H}}(G)$. 
Figure 3: Illustration for two blocks $B_j$ and $B_k$ ($k < j < i$) pre-identical to a block $B_i$.

Given an integer $n \geq 2$, we design an algorithm $\texttt{GENERATE}(n)$ which generates all canonical embeddings of graphs in $\mathcal{H}$ containing at most $n$ vertices.

**Algorithm $\texttt{GENERATE}(n)$**

Input: An integer $n \geq 2$.

Output: All canonical embeddings of graphs in $\mathcal{H}$ containing at most $n$ vertices.

begin

Create an embedding $G$ with exactly one block $B_1$ by setting $B_1$ to be the seed block $\tilde{B} \in \mathcal{B}$;

$C(B_1) := \emptyset$; /* $C(B)$ denotes the competitor of $B$ */

Output $G$; $\texttt{GEN}(G)$

end.

After creating a new block equivalent to the seed block $\tilde{B} \in \mathcal{B}$ as the first block $B_1$ in an canonical embedding $G$, we generate all canonical child-embeddings $G'$ of $G$ by the following recursive procedure $\texttt{GEN}(G)$.

**Procedure $\texttt{GEN}(G)$**

Input: A canonical embedding $G$ with at most $n$ vertices.

Output: All descendent-embeddings of $G$ containing at most $n$ vertices.

begin

/* Let $\pi(G) = [B_1, B_2, \ldots, B_K]$, and let $(B^1, B^2, \ldots, B^p)$ be the spine of $G$,
where $B^p = B_K$ is the tip-block of $G$ */

LOWESTBLOCK;

/* Let $B^h$ be the lowest block in the spine to which a new block can be appended */

if $|V(G)| + |V'(\tilde{B})| \leq n$ then

for $i = 1, 2, \ldots, h$ do

APPENDSEED

endfor

endif;

if $h = p$ then EXPANDTIP endif

end.
Supposing that a canonical embedding $G$ is obtained, we give an outline of GEN($G$). We easily see that a child-embedding $G'$ of $G$ is obtained by appending a new block $B$ to a vertex in a block in the spine of $G$ or by extending the tip-block $B^p$ of $G$ to its child $B \in C_B(B^p)$. We first compute the lowest block $B^h$ in the spine of $G$ that contains a vertex to which a new block can be appended to generate a canonical child-embedding of $G$. Hence GEN($G$) consists of three tasks: LOWESTBLOCK: the task of finding the lowest block $B^h$, APPENDSEED: the task of appending new blocks to all blocks $B^i$, $i \leq h$ in the spine, and EXPANDTOP: the task of extending the tip-block $B^p$ of $G$ to each of all children $B \in C_B(B^p)$.

To facilitate finding the lowest block $B^h$ in LOWESTBLOCK, we introduce “competitors” of blocks in an embedding. We define the competitor of a block $B_i$ to be the block $B_j$ pre-identical to $B_i$ which has the smallest index $j$ ($< i$) among all blocks pre-identical to $B_i$. A block $B_i$ has no competitor if no block $B_j$, $j < i$ is pre-identical to $B_i$.

Let $G'$ be the embedding obtained from a canonical embedding $G$ by appending a new block $B$ which is equivalent to the seed block $B \in E$ to a vertex $v \in V'(B^i)$ of a block $B^i$ in the spine of $G$. We consider when $G'$ remains canonical. Since $G$ needs to be the parent-embedding of $G'$, the new block $B$ in $G'$ needs to be the tip-block of $G'$. To obtain a correct child-embedding $G'$ from $G$, the vertex $v$ must satisfy key($v$) $< \min\{key(u) \mid V_{cut}(B^j)\}$, where $\min\{key(u) \mid V_{cut}(B^p)\} = \infty$ for the tip-block $B^p$ of $G$.

**Lemma 7** Let $B_i$ and $B_j$ ($j < i$) be blocks in the spine of a canonical embedding $G$. Assume that the child-embedding $G'_j$ is obtained from $G$ by appending a new seed block to a vertex $u \in V'(B^j)$. Then the child-embedding $G'_j$ obtained from $G$ by appending a seed block to any vertex $v \in V'(B^j)$ satisfying key($v$) $< \min\{key(u) \mid V_{cut}(B^j)\}$ is canonical.

**Proof.** Since $d(G'_j) < d(G'_i)$, we see that $\gamma'(B)$ of the new block $B$ appended to $v$ in $G'_j$ is smaller than $\gamma'(B)$ of $B$ appended to $u$ in $G'_i$. Hence only the right hand side of each of the inequalities in Lemmas 2 and 3 for blocks in the spine of $G'_j$ can decrease by replacing the position of the new block, indicating that $G'_j$ remains canonical.

Consider the block $B^h$ with the smallest $h$, called the lowest block, to which the seed block can be appended to obtain a canonical child-embedding $G'$, and the maximum key endkey$^h$ of a vertex $v \in V'(B^h)$ with key($v$) $\leq$ endkey$^h$ to which the seed block can be appended to obtain a canonical child-embedding $G'$.

For two incomparable blocks $B_i$ and $B_j$ ($i < j$), let $rblock(B_i, B_j)$ be the ancestor-block $B_h$ of $B_j$ with $r(B_h) = lca(B_i, B_j)$ if $lca(B_i, B_j)$ is a vertex; let $rblock(B_i, B_j)$ be the first right child-block of block $lca(B_i, B_j)$ otherwise.

**Lemma 8** Let $G$ be a canonical embedding, and denote $\pi(G) = [B_1, B_2, \ldots, B_K]$, and let $(B^1, B^2, \ldots, B^p)$ be the spine of $G$, where $B^p = B_K$ is the tip-block of $G$. Assume that $B^p$ has the competitor $B_j$ with $\gamma'(B_j) \simeq \gamma'(B_K)$. Let $B_l$ be the parent-block of $B_{j+1}$ in $G$, and let $B^* = B_{j+1}$ in the spine with $d(B^*) = d(B_l)$.

(i) If $\gamma'(B_j) = \gamma'(B_K)$ and $B_{j+1}$ is a left child-block of the symmetric block $lca(B_j, B_K)$, then the lowest block $B^h$ is given by $B^*$ and endkey$^h = (1, t(r(B_{j+1})))$ (see Fig. 4(a));

(ii) If $\gamma'(B_j) \simeq \gamma'(B_K)$ and $B_{j+1}$ is the first right child-block of the symmetric block $lca(B_j, B_K)$, then the lowest block $B^h$ is given by the parent-block of $B^*$ and endkey$^h = key(r(B^*))$ (see Fig. 4(b),(c)); and

(iii) In the other case than (i)-(ii), $B^h$ is given by $B^*$ and endkey$^h = key(r(B_{j+1}))$ (see Fig. 4(d)-(f)).

**Proof.** We can observe that the case where $B^p$ has the competitor $B_j$ with $\gamma'(B_j) \simeq \gamma'(B_K)$ has the following six subcases: (a) $B_{j+1}$ is a left child-block of symmetric block $lca(B_j, B_K) = B^* = B_l$ (see Fig. 4(a));
Lemma 9 For a canonical embedding $G$, let $\pi(G) = [B_1, B_2, \ldots, B_K]$, and let $(B^1, B^2, \ldots, B^p)$ be the spine of $G$, where $B^p = B_K$ is the tip-block of $G$. Assume that $B^p$ has no competitor $B_j$ with $\gamma'(B_j) \simeq \gamma'(B_K)$. Then the lowest block $B^h$ is given by the tip-block $B^p$ and endkey$^h = \infty$. 

(b) $B_{j+1}$ is the first right child-block of symmetric block $lca(B_j, B_K) = B^* = B_1$, and $B_j$ and $B_K$ are right and left child-blocks of $lca(B_j, B_K)$ (see Fig. 4(b));

(c) $B_{j+1}$ is the first right child-block of symmetric block $lca(B_j, B_K) = B^* = B_1$, and both $B_j$ and $B_K$ are not child-blocks of $lca(B_j, B_K)$ (see Fig. 4(c));

(d) $B_{j+1}$ is a descendant-block of a left child-block of symmetric block $lca(B_j, B_K)$ (see Fig. 4(d));

(e) $B_{j+1}$ is a descendant-block of a left child-block of vertex $lca(B_j, B_K)$ (see Fig. 4(e)); and

(f) $B_{j+1}$ is the child-block $rblock(B_j, B_K)$ of vertex $lca(B_j, B_K)$ (see Fig. 4(f)).

Let $B^h$ and endkey$^h = \text{key}(r(B_{j+1}))$ be the block and the key value determined by the lemma. Then we see that the block $lca(B_j, B_K)$ or $rblock(B_j, B_K)$ is no longer left-side-heavy or left-sibling-heavy if a new block $B$ is appended at a vertex $u$ such that $u \in V'(B^h)$ with key$(u) > \text{endkey}^h$ or $u \in V'(B^i)$ with $i > h$.

We next show that the embedding $G'$ obtained from $G$ by appending a new seed block $B$ to the vertex $u \in V'(B^h)$ with key$(u) = \text{endkey}^h$ is canonical, which proves that $B^h$ is the lowest block and endkey$^h$ is the maximum key in $V'(B^h)$ by Lemma 7. We consider case (a) (the other cases can be treated analogously). Assume that $G'$ is not canonical. Then $G'$ has a block $B_a$ which is not left-sibling-heavy or is not left-side-heavy. Since we see that $B_l = B^h = lca(B_j, B_K)$ remains left-side-heavy in $G'$, we have $a < l$. Then the new tip-block $B'$ has a pre-identical block $B_l$ in $G'$. This means that block $B_{t-1}$, $t - 1 < j$, is pre-identical to $B_K$, contradicting that $B_j$ with $t - 1 < j$ is the competitor of $B_K$. 

![Figure 4: Illustration for the six subcases of the case where the tip-block $B_K = B^p$ has the competitor $B_j$ with $\gamma'(B_j) \simeq \gamma'(B_K)$.

(a) $B^h = lca(B_j, B_K)$, (b) $lca(B_j, B_K) = B^* = B_1$, (c) $lca(B_j, B_K) = B^* = B_1$, (d) $lca(B_j, B_K) = B^* = B_1$, (e) $lca(B_j, B_K) = B^* = B_1$, (f) $lca(B_j, B_K) = B^* = B_1$]
Proof. By Lemma 7, it suffices to show that the embedding $G'$ obtained from $G$ by appending a new seed block $B$ to the vertex $u \in V'(B^h)$ with the maximum key is canonical. Assume that $G'$ is not canonical. Then $G'$ has a block $B_0$ which is not left-sibling-heavy or is not left-side-heavy. Then the new tip-block $B'$ has a pre-identical block $B_t$ in $G'$. This means that block $B_{t-1}$ is pre-identical to $B_K$, contradicting that $B_K$ has no competitor in $G$.

Task LOWESTBLOCK is attained by computing the lowest block $B^h$ and the the maximum key endkey$^h$ according to Lemmas 8 and 9.

LOWESTBLOCK
if $\gamma'(C(B_K)) \approx \gamma'(B_K)$ then /* $B_j = C(B_K)$ in $\pi(G)$ */
  Let $B_t$ be the parent-block of $B_{t+1}$ in $G$;
  Let $B^*$ be the block in the spine with $d(B^*) = d(B_t)$;
  if lca($B_j, B_K$) = $B^*$ then
    $B^h := B^*$; endkey$^h$ := (1, $\ell(r(B_{j+1}))$)
  else if $B_{j+1}$ is the first right child-block of $B^*$ = lca($B_j, B_K$) then
    Let $B^h$ be the parent-block of $B^*$; endkey$^h$ := key($r(B^*)$)
  endif endif
else
  $B^h := B^*$; endkey$^h$ := key($r(B_{j+1})$)
endif endif
if $\gamma'(C(B_K)) \not\approx \gamma'(B_K)$ then $B^h := B^p$; endkey$^h$ := $\emptyset$

We are ready to examine when the embedding $G'$ obtained from $G$ by extending the tip-block $B^p$ to one of its child $B \in C_B(B^p)$ remains canonical.

Lemma 10 Let $G'$ be the embedding obtained from a canonical embedding $G$ by expanding the tip-block $B^p$ to a child $B \in C_B(B^p)$. Then $G'$ is not canonical if and only if $B^p$ has the competitor $B_j$ in $G$ and $\gamma(B) > \gamma(B_j)$ holds.

Proof. (i) If part: Assume that $B^p$ has the competitor $B_j$ and $\gamma(B) > \gamma(B_j)$ holds. If lca($B_j, B^p$) is a block $B_t$, then we see that $B_t$ is not left-side-heavy in $G'$. Otherwise if lca($B_j, B^p$) is a vertex $v$, then there are two consecutive siblings $B^j_B, B^j_{B''} \in BS[v]$ such that $B^j_B$ and $B^j_{B''}$ are ancestor-blocks of $B^j_B$ and $B^p$, indicating that $B^j_B$ is not left-sibling-heavy in $G'$.
(ii) Only if part: Assume that $G'$ is not canonical. Since $G$ is canonical, we see that all blocks $B'$ that are not left-side-heavy or left-side-heavy in $G'$ belong to the spine of $G$. Let $B_k$ be such a block $B'$.

First consider the case where $B_k$ is not left-side-heavy in $G'$. Then the left sibling $B^h_k \in BS[v]$ of $B_k$ at the root $v = r(B_k)$ has a descendant-block $B_c$ which is pre-identical to $B^p$ in $G'$ and satisfies $\gamma(B) > \gamma(B_c) \geq \gamma(B^p)$ and $\gamma'(B_c) \geq \gamma'(B^p)$ holds. Hence by definition, $B^p$ has the competitor $B_b$ with $b \leq c$. Since $b = c$ implies the lemma, we derive a contradiction assuming $b < c$. Since $b < c$ and $B_b$ is pre-identical to $B^p$, we have $(d(B_b), key(r(B_b))) = (d(B^p), key(r(B^p)))$ (note that $B_b$ and $B^p$ cannot share the same parent-block due to the block $B_c$). By Lemma 6, it holds $\gamma'(B_c) \geq \gamma'(B_b) \geq \gamma'(B^p)$. Hence, $(d(B_b), key(r(B_b))) = (d(B_c), key(r(B_c))) = (d(B^p), key(r(B^p)))$ implies that $\gamma(B_c) \geq \gamma(B_b) \geq \gamma(B^p)$. From this and $\gamma(B) > \gamma(B_c) \geq \gamma(B^p)$, we obtain $\gamma(B) > \gamma(B_c) = \gamma(B_b) = \gamma(B^p)$, as required.

Next consider the case where $B_k$ is a symmetric block which is not left-side-heavy in $G'$. Then $B^p$ is a descendant-block of a right child-block of $B_k$ and there is descendant-block $B_c$ of a left child-block of $B_k$ which is pre-identical to $B^p$ in $G$ and satisfies $\gamma(B) > \gamma(B_c) \geq \gamma(B^p)$ and $\gamma'(B_c) \geq \gamma'(B^p)$ holds.

(1) If $\gamma'(C(B_K)) \approx \gamma'(B_K)$ then /* $B_j = C(B_K)$ in $\pi(G)$ */
  Let $B_t$ be the parent-block of $B_{t+1}$ in $G$;
  Let $B^*$ be the block in the spine with $d(B^*) = d(B_t)$;
  if lca($B_j, B_K$) = $B^*$ then
    $B^h := B^*$; endkey$^h$ := (1, $\ell(r(B_{j+1}))$)
  else if $B_{j+1}$ is the first right child-block of $B^*$ = lca($B_j, B_K$) then
    Let $B^h$ be the parent-block of $B^*$; endkey$^h$ := key($r(B^*)$)
  endif endif
else
  $B^h := B^*$; endkey$^h$ := key($r(B_{j+1})$)
endif endif
if $\gamma'(C(B_K)) \not\approx \gamma'(B_K)$ then $B^h := B^p$; endkey$^h$ := $\emptyset$
$B^p$ are child-blocks of $B_K$). By definition, $B^p$ has the competitor $B_p$ with $b \leq c$. Since $b = c$ implies the lemma, we derive a contradiction assuming $b < c$. Since $b < c$ and $B_p$ is pre-identical to $B^p$, we have $(d(B_b), \text{key}(r(B_b))) = (d(B^p), \text{key}(r(B^p)))$. By Lemma 6, it holds $\gamma'(B_c) \geq \gamma'(B_b) \geq \gamma'(B^p)$. Again this and $\gamma(B) > \gamma(B_c) \geq \gamma(B^p)$ imply $\gamma(B) > \gamma(B_c) = \gamma(B_b) = \gamma(B^p)$, as required.

By Lemma 10, if $B^p$ has the competitor $B_j$ with $\gamma'(B_j) \simeq \gamma'(B^p)$, then the tip-block $B^p$ cannot be expanded to generate a canonical embedding. In this case, the lowest block $B^h$ is not equal to $B^p$ by Lemma 8. On the other hand, $B^p$ is the lowest block $B^h$ by Lemma 9. Hence we try to expand the tip-block $B^p$ only when $B^h = B^p$. Based on the above observation, a procedure for EXPANDTIP is described as follows.

**EXPANDTIP**

Let $B_{\text{min}} := \bar{B}$ and $B_{\text{max}} := C(B_K)$ (let $B_{\text{max}} := \infty$ if $C(B_K) := \emptyset$);

while $B := \text{NEXTMINCHILD}(B_K, B_{\text{min}}, B_{\text{max}}) \neq \emptyset$ and $|V(G)| + |V'(B)| \leq n$ do

\[ B := \text{NEXTMINCHILD}(B_K, B_{\text{min}}, B_{\text{max}}); \]
Let $G'$ be the embedding obtained from $G$ by replacing $B_K$ with $B$, and output $G'$ (or the difference between $B_K$ and $B$);

GEN($G'$);

$B_{\text{min}} := B$
endwhile

To append a new block to the current embedding $G$, we need to know all vertices to which a new block can be appended one by one.

A procedure for APPENDSEED can be described as follows. Let $B^0$ denote an imaginary block which is the parent-block of $r_G = r(B^1)$ such that $V'(B^0) = \{r_G\}$ for notational convenience.

**APPENDSEED**

if $i < h$ then endkey$^i := \text{key}(r(B^{i+1}))$ for the root $r(B^{i+1})$ of block $B^{i+1}$ endif;

currentkey := $-\infty$;

while NEXTVERTEX($B^i$, currentkey) $\neq \emptyset$ do

(v, key(v)) := NEXTVERTEX($B^i$, currentkey);
Create a new block $B$ which is equivalent to seed block $\bar{B}$;
Let $G'$ be the embedding obtained from $G$ by appending block $B$ to $v$;
Compute the competitor $C(B)$ of the new block $B$, lca($C(B), B$) and rblock($C(B), B$) according to Cases-C1 and C2;
Output $G'$ (or $B$ and $v$);

GEN($G'$);

currentkey := $\text{key}(v)$;

if currentkey = endkey$^i$ then currentkey := $\infty$

/* This terminates the while-loop by NEXTVERTEX($B^i, \infty$) = $\emptyset$ */
endif
endwhile /* no vertex in $B^i$ is left for appending a new block */

We can compute the competitor $C(B)$ of the new block in APPENDSEED in $O(1)$ time if we also maintain data lca($C(B), B$) and rblock($C(B), B$).

We assume that the set of vertices in $V'(B)$ of a block $B \in B$ is stored in a linked list $LIST(B)$ in the decreasing order with respect to their levels $\ell$, and that the following procedure NEXTVERTEX of reporting the current vertex in $LIST(B)$ is available.

**Procedure** NEXTVERTEX($B, \kappa$)
Input: A block $B$ and a key value $\kappa \in \{1, 2, 3\} \times \mathbb{Z} \cup \{-\infty, \infty\}$, where $\mathbb{Z}$ denotes the set of integers.
Output: The vertex name $u$ and key $\text{key}(u) = (\text{side}(u), \ell(u))$ of the vertex next to the vertex $v \in V(B)$ with $\text{key}(v) = \kappa$ in a list $\text{LIST}(B)$ of vertices to which a block can be attached, where we choose such a vertex $u$ from $V_2(B)$, $V_j(B)$, $V_1(B)$ in this order and the first such vertex is chosen when $\kappa = -\infty$; return $0$ if no such a nonroot vertex $v$ of $B$ exists or $\kappa = \infty$.

We can maintain the cell in $\text{LIST}(B)$ that was accessed last by a pointer so that the next cell can be accessed in constant time.

We also assume that a procedure $\text{NEXTMINCHILD}$ for returning a block $B' \in B$ with $\gamma(B_{\min}) < \gamma(B') \leq \gamma(B_{\max})$ for given blocks $B_{\min}$ and $B_{\max}$ is available.

**Procedure** $\text{NEXTMINCHILD}(B, B_{\min}, B_{\max})$

Input: Blocks $B$, $B_{\min}$ and $B_{\max}$, where possibly $B_{\max} = \infty$.
Output: The block $B' \in \mathcal{G}(B)$ with the minimum $\gamma(B')$ such that $\gamma(B_{\min}) < \gamma(B') \leq \gamma(B_{\max})$ (if any) or $B' = 0$ if no such $B'$ exists, where we treat $\gamma(B_{\max})$ with $B_{\max} = \infty$ as $\infty$.

**How to Compute Competitors** For each block $B_i \in \pi(G)$, $i = 1, 2, \ldots, K$ in this order, we can set the competitor of a block $B_i$ to be the block $B_j$ which satisfies one of the next cases holds, where we also compute $\text{lca}(B_i, B_j)$ and $\text{rblock}(B_i, B_j)$:

**Case-C1.** $i \geq 2$ and the previous block $B_{i-1}$ of $B_i$ has a competitor $B_{j-1}$ and it holds $\text{lca}(B_i, B_j) = \text{lca}(B_{i-1}, B_{j-1})$:

(a) $\text{lca}(B_i, B_j)$ is a vertex and $\gamma'(B_{i-1}) = \gamma'(B_{j-1})$ holds: Then the competitor of $B_i$ is given by $B_j$.

(b) $\text{lca}(B_{i-1}, B_{j-1})$ is a symmetric block, $B_{i-1}$ and $B_{j-1}$ are not child-blocks of block $\text{lca}(B_i, B_j)$, and $\gamma'(B_{i-1}) = \gamma'(B_{j-1})$: Then the competitor of $B_i$ is given by $B_j$.

(c) $\text{lca}(B_{i-1}, B_{j-1})$ is a symmetric block, $B_{i-1}$ and $B_{j-1}$ are child-blocks of block $\text{lca}(B_i, B_j)$, and $\gamma'(B_{i-1}) = \gamma'(B_{j-1})$: Then the competitor of $B_i$ is given by $B_j$.

In each of (a)-(c), we set $\text{lca}(B_i, B_j) := \text{lca}(B_{i-1}, B_{j-1})$ and $\text{rblock}(B_i, B_j) := \text{rblock}(B_{i-1}, B_{j-1})$.

**Case-C2.** $B_i$ has no such previous block $B_{i-1}$ in Case-C1:

(a) $B_i$ has a left sibling $B_j \in \text{BS}[v]$ at $v = r(B_i)$: Then the competitor of $B_i$ is given by $B_j$. We set $\text{lca}(B_i, B_j) := v$ and $\text{rblock}(B_i, B_j) := B_i$.

(b) $B_i$ has no left sibling $B_j \in \text{BS}[v]$ at $v = r(B_i)$, $B_i$ has the parent-block $B_t$ which has a left child-block, and $B_i$ is the first right child-block of $B_t$: Then the competitor of $B_i$ is given by the left first child-block $B_j$ of $B_t$. We set $\text{lca}(B_i, B_j) := B_t$ and $\text{rblock}(B_i, B_j) := B_i$.

**Lemma 11** In a canonical embedding $G$, the competitor of block $B_t$ is correctly obtained in Cases-C1 and C2, if any, if the competitors of all blocks $B_i$, $t < i$ have been obtained.

**Proof.** If $B_t$ has a left sibling at $v = r(B_t)$, then $B_t$ has a competitor. Note that a block $B$ which has a right child-block must have a left child-block in a canonical embedding $G$, since otherwise $B$ is not left-side-heavy. Hence if $B_t$ is the first right child-block of its parent-block $B_i$, then $B_t$ has a left child-block and thereby $B_t$ has a competitor.

(i) Assume that there is no block pre-identical to $B_t$. We show that no competitor is given to $B_t$ in Case-C1 and C2. Since $B_t$ in Case-C2 is pre-identical to $B_i$, we consider Case-C1(a), i.e., $B_{i-1}$ has the competitor $B_{j-1}$ such that $\text{lca}(B_j, B_j) = \text{lca}(B_{i-1}, B_{j-1})$ is a vertex $v$ and $\gamma'(B_{j-1}) = \gamma'(B_{i-1})$ holds (subcases (b) and (c) can be treated analogously). By definition of competitors, we have $\text{ps}(v, B_{i-1}) = \text{ps}(v, B_{j-1})$. Since $\gamma'(B_{j-1}) = \gamma'(B_{i-1})$ holds, it holds $\text{ps}(v, B_j) = [\text{ps}(v, B_{j-1}), \gamma'(B_{j-1})] = [\text{ps}(v, B_{i-1})$, $\gamma'(B_{i-1})]$.
We obtain

\[(B_{k-1}, T(n)) = \psi(B_{k-1}, T(n)) = \psi(B_{i-1}, T(n)) = (B_{i-1}, T(n)) \simeq (B_{i-1}, \gamma'(B_{i-1})中断).\]

This, however, implies that \(B_j\) is pre-identical to \(B_i\), contradicting that there is no block pre-identical to \(B_i\). Therefore, no competitor is assigned to \(B_i\).

(ii) Assume that there is a block \(B_t, t < i\) pre-identical to \(B_i\). Let \(t\) be the minimum index for such block \(B_t\). We show that if \(B_t\) is the left sibling in \(B_{S[v]} \at v = r(B_i)\), then no competitor is assigned to \(B_t\) in Case-C1, which implies that \(B_t\) is assigned to \(B_i\) as the competitor of \(B_t\) in Case-C2(a).

If a block \(B_j\) in Case-C1 is assigned to such \(B_i\) in Case-C1, then we see that \(B_j\) is pre-identical to \(B_i\), and \(j < t\) holds, contradicting the choice of \(B_t\). We can treat the case where \(B_t\) and \(B_i\) are the first left- and right-blocks of a block anomalously.

Assume that \(B_t\) and \(B_i\) do not satisfy each of conditions (a) and (b) in Case-C2. In this case, the preceding block \(B_{i-1}\) of \(B_i\) is pre-identical to the preceding block \(B_{i-1}\) of \(B_i\). Hence if the competitor of \(B_{i-1}\) is \(B_{i-1}\), then \(B_t\) is assigned to \(B_i\) as its competitor in Case-C1, as required. We derive a contradiction by assuming that the competitor of \(B_{i-1}\) is a block \(B_{k-1}\) with \(k - 1 < t - 1\). By Lemma 6 and \(\gamma'(B_{t-1}) = \gamma'(B_{i-1}),\) we have \(\gamma'(B_{k-1}) \simeq \gamma'(B_{i-1}).\) This, however, means that \(B_k\) is pre-identical to \(B_i\), contradicting the choice of \(B_t\).

Finally we consider the entire algorithm GENERATE. For the correctness of GENERATE, we only need to show that, when \(\text{GEN}(G)\) terminates a recursive call to avoid generating \(G'\) with more than \(n\) vertices, all descendant-embeddings of \(G\) with at most \(n\) vertices have been generated. In \(\text{GEN}(G)\), task \(\text{APPENDSEED}\) is executed only when \(|V(G)| + |V'(B)| \leq n\). We see that, if \(|V(G)| + |V'(B)| > n\), then no child-embedding \(G'\) of \(G\) obtained by appending the seed block can have an embedding with at most \(n\) vertices due to the monotonicity (SS) of \(\gamma\). Similarly, \(\text{EXPANDTIP}\) terminates expansion of the tip-block once the new expanded block \(B\) satisfies \(|V(G)| + |V'(B)| > n\). In this case, no child-embedding \(G'\) of \(G\) obtained by expanding the tip-block \(B'\) to any other unseen children \(B' \in C\) because \(\gamma(B') > \gamma(B)\) holds by the listing order of \(\text{NEXTMINCHILD}\) and thereby \(|V(B')| \geq |V(B)| \geq n\) holds by the monotonicity (S4) of \(\gamma\).

It is not difficult to implement \(\text{GENERATE}(n)\) so that each new embedding can be generated in \(O(\Delta)\) time and \(O(n)\) without including the time and space complexity of procedures \(\text{NEXTVERTEX}\) and \(\text{NEXTMINCHILD}\), where \(\Delta\) denotes the maximum size between two consecutive outputs. Let \(T(n)\) and \(S(n)\) denote the time and space complexities of procedures \(\text{NEXTVERTEX}\) and \(\text{NEXTMINCHILD}\). Then we see that all rooted graphs in \(\mathcal{H}\) can be generated by \(\text{GENERATE}(n)\) in \(O(T(n))\) time in average and in \(O(S(n) + n)\) time, where \(\Delta = O(T(n))\) is assumed. We can reduce the worst case of time delay between two consecutive outputs to \(O(T(n))\) using the technique of changing the timing of outputs (e.g., [8, 7, 9]) so that a canonical embedding \(G\) at an odd (resp., even) depth in the family tree \(\mathcal{F}_\mathcal{H}\) is output before (resp., after) generating any child of \(G\).

**Theorem 12** Let \(B\) be a class of blocks which admits signature \(\gamma\) monotone with respect to the number of vertices. Then all canonical embeddings of rooted graphs in a class \(\mathcal{H}\) over \(B\) can be generated in \(O(S(n) + n)\) space and in \(O(T(n))\) time per output.

### 6 Concluding Remarks

In this paper, we introduce a framework for generating rooted graphs which consists of representations of biconnected components with reflective symmetries, called blocks. Our framework delivers an algorithm for generating all graphs in such a class of graphs in constant time per output if two procedures \(\text{NEXTVERTEX}\) and \(\text{NEXTMINCHILD}\) for the class of blocks are designed so that they run in in constant time per output. Recently, we have designed an algorithm that generates all rooted *biconnected planar*
graphs with internally triangulated faces in $O(1)$ time per output [12, 13]. The algorithm also provides procedures NEXTVERTEX and NEXTMINCHILD that run in $O(1)$ time. Hence Theorem 12 implies that all rooted connected planar graphs with internally triangulated faces can be generated in $O(1)$ time per output.

In this paper, we have treated a class of biconnected components that admits symmetry whose order is at most 2. It seems possible to extend our framework to symmetry of blocks with a higher order such a rotational symmetry with order $k \geq 2$. It is also our future work to provide a new framework for rooted graphs which consists of representations of triconnected components with reflectional symmetries.

References