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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], Fujiwara 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 then 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 $A \sqsupseteq B$ 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 label 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 ψ 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* ℓ 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 $v \in V_1(B)$.

Let $\mathcal{B}$ denote a set of such blocks. More formally, we assume that a parent-child graph relationship $(\mathcal{P}_\mathcal{B}, \mathcal{C}_\mathcal{B})$ 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, $\mathcal{P}_\mathcal{B}(B')$ denotes a block $B' \in \mathcal{B}$ that is defined as the parent of B, and $\mathcal{C}_\mathcal{B}(B')$ denotes the set of children of B', i.e., blocks B'' with $B' = \mathcal{P}_\mathcal{B}(B'')$. Also assume that there exists *signature* γ 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, γ is called *monotone* with respect to the number of vertices if the followings hold: (S4) for any two blocks $B', B'' \in \mathcal{C}_{\mathcal{B}}(B)$, $B \in \mathcal{B}$, 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 $B' \in \mathcal{C}_{\mathcal{B}}(B)$, and $|V(B')| > |V(B)|$, for all $B' \in \mathcal{C}_{\mathcal{B}}(\tilde{B})$.

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* $\mathrm{lca}(B_1, B_2)$ 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 $\mathrm{lca}(B_1, B_2)$ to be block B_1. If $B_1 \neq B_2$ and B_1 is an ancestor-block of B_2, then $\mathrm{lca}(B_1, B_2)$ 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.

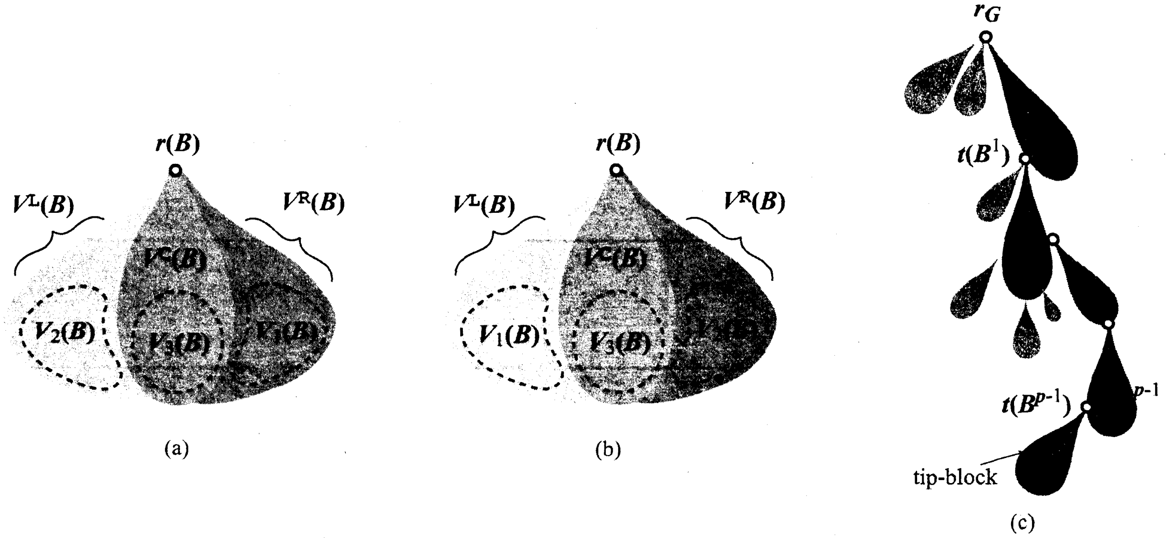

Figure 1: (a), (b) Two left/right-assignments of $V^{\mathrm{R}}(B)$ and $V^{\mathrm{L}}(B)$ to $V_2(B)$ and $V_3(B)$ of a symmetric block B; (c) Spine $B^1, B^2, \ldots, B^p$ of an embedding G.

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* $V^{\mathrm{C}}(B)$, $V^{\mathrm{L}}(B)$ and $V^{\mathrm{R}}(B)$ as follows. For the vertex set $V_3(B)$, we always set $V^{\mathrm{C}}(B) = V_3(B)$. For the vertex sets $V_1(B)$ and $V_2(B)$, there are two choices, either $V^{\mathrm{L}}(B) = V_1(B)$, $V^{\mathrm{R}}(B) = V_2(B)$ or $V^{\mathrm{L}}(B) = V_2(B)$, $V^{\mathrm{R}}(B) = V_1(B)$, as shown in Fig. 1(a) and (b). For an asymmetric block $B \in \mathcal{B}$, let $V^{\mathrm{C}}(B) = V(B)$ and $V^{\mathrm{L}}(B) = V^{\mathrm{R}}(B) = \emptyset$. For each vertex $v \in V(B)$, define the *side* $\mathrm{side}(v)$ of v in B to be the index i such that $v \in V_i(B)$. For convenience, we call a vertex in $V^{\mathrm{L}}(B)$ (resp., $V^{\mathrm{R}}(B)$ and $V^{\mathrm{C}}(B)$) *left* (resp., *right* and *central*). We assume that $V^{\mathrm{C}}(B)$, $V^{\mathrm{L}}(B)$ and $V^{\mathrm{R}}(B)$ 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 ϕ 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 σ 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 $V_{\mathrm{cut}}(B)$ denote the set of cut-vertices of $v \in V'(B)$. Let $V^{\mathrm{L}}_{\mathrm{cut}}(B) = V_{\mathrm{cut}}(B) \cap V^{\mathrm{L}}(B)$. Similarly for $V^{\mathrm{R}}_{\mathrm{cut}}(B)$ and $V^{\mathrm{C}}_{\mathrm{cut}}(B)$. For a block B, a child-block B' of B is called a *left* (resp., *right* and *central*) child-block if $r(B') \in V^{\mathrm{L}}(B)$ (resp., $r(B') \in V^{\mathrm{R}}(B)$ and $r(B') \in V^{\mathrm{C}}(B)$), where $V^{\mathrm{L}}(B) = V^{\mathrm{R}}(B) = \emptyset$. 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 ℓ.

We define the *tip* $t(B)$ of a block B with $V_{\mathrm{cut}}(B) \neq \emptyset$ in an embedding G to be the vertex $v \in V_{\mathrm{cut}}(B)$ with the smallest key. In other words, *tip* $t(B)$ is chosen as follows:
(1) $V^{\mathrm{R}}_{\mathrm{cut}}(B) \neq \emptyset$: Define $t(B)$ to be the right vertex $v \in V^{\mathrm{R}}_{\mathrm{cut}}(B)$ with the smallest $\ell(v)$;
(2) $V^{\mathrm{R}}_{\mathrm{cut}}(B) = \emptyset$ and $V^{\mathrm{L}}_{\mathrm{cut}}(B) \neq \emptyset$: Define $t(B)$ to be the left vertex $v \in V^{\mathrm{L}}_{\mathrm{cut}}(B)$ with the smallest $\ell(v)$; and
(3) $V^{\mathrm{R}}_{\mathrm{cut}}(B) = V^{\mathrm{L}}_{\mathrm{cut}}(B) = \emptyset$, and $V^{\mathrm{C}}_{\mathrm{cut}}(B) \neq \emptyset$: Define $t(B)$ to be the central vertex $v \in V^{\mathrm{C}}_{\mathrm{cut}}(B)$ with the smallest $\ell(v)$.

For a block B such that $V_{\mathrm{cut}}(B) \neq \emptyset$, the *successor* of B is defined to be the rightmost block in $BS[t(B)]$. The *spine* 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 $\mathcal{P}_{\mathcal{H}}(G)$ 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 $\mathcal{P}_{\mathcal{H}}(G)$ is defined to be the embedding obtained by replacing B with its parent $\mathcal{P}_{\mathcal{B}}(B)$.
2. Otherwise, $\mathcal{P}_{\mathcal{H}}(G)$ 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 $\mathcal{P}^i_{\mathcal{H}}(G)$, $i = 0, 1, \ldots, K-1$ denote the embedding $\mathcal{P}_{\mathcal{H}}(\mathcal{P}^{i-1}_{\mathcal{H}}(G))$. Let $\pi(G) = (B_1, B_2, \ldots, B_K)$, where B_i is the tip-block of $\mathcal{P}^{K-i}_{\mathcal{H}}(G)$, 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

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

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

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

where $\delta(r(\mathcal{P}_{\mathcal{B}}(B_K))) = \delta(r(B_K))$.

For two indices i and j $(i \le j)$, 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 $B_i, B_{i+1}, \ldots, B_j$ that appear in this order in $\pi(G)$. and let $\sigma(G(B); G)$ denote $\sigma_{i,j}(G)$. Then signature σ 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_i denote the embedding induced from G by the first i blocks in $\pi(G)$, i.e., G_i 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 with $\sigma(G_{j+1}) = \sigma_{j+1}$. 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 σ_{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 suffices 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 such one 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 ℓ. 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 $B = B_i, B_{i+1}, \ldots, B_j$ 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 $\sigma(G) \ge \sigma(G')$ holds for the embedding G' obtained from G by exchanging the order of B'_{i-1} and $B'_i = B$ 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 $i \ge 2$ if and only if $\sigma(G(B'_{i-1}); G) \ge \sigma(G(B'_i); G)$ 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 $\sigma(G(B'_i);G') = \sigma(G(B'_i);G)$ and $\sigma(G(B'_{i-1});G') = \sigma(G(B'_{i-1});G)$. Hence $\sigma(G) \geq \sigma(G')$ holds if and only if

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

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

$$[\sigma(G(B'_{i-1});G),\sigma(G(B'_i);G)] > [\sigma(G(B'_i);G),\sigma(G(B'_{i-1});G)], \tag{1}$$

and that $\sigma(G(B'_i);G) > \sigma(G(B'_{i-1});G)$ implies $[\sigma(G(B'_i);G),\ \sigma(G(B'_{i-1});G)] > [\sigma(G(B'_{i-1});G),\ \sigma(G(B'_i);G)]$. By symmetry, it is sufficient to show the former.

Assume that $\sigma(G(B'_{i-1});G) > \sigma(G(B'_i);G)$. If "$\sigma(G(B'_{i-1});G) \gg \sigma(G(B'_i);G)$" or "$|\sigma(G(B'_{i-1});G)| = |\sigma(G(B'_i);G)|$ and $\sigma(G(B'_{i-1});G) \sqsupset \sigma(G(B'_i);G)$" holds, then we have $[\sigma(G(B'_{i-1});G),\sigma(G(B'_i);G)] > [\sigma(G(B'_i);G'),\sigma(G(B'_{i-1});G')]$. Then we consider the case where $\sigma(G(B'_{i-1});G) \sqsupset \sigma(G(B'_i);G)$ and $|\sigma(G(B'_{i-1});G)| > |\sigma(G(B'_i);G)|$. In this case, the first code $\gamma'(B_a)$ in $\sigma(G(B'_{i-1});G)$ is compared with the $(|\sigma(G(B'_i);G)|+1)$st code $\gamma'(B_b)$ in $\sigma(G(B'_{i-1});G)$.

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

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

For a block B, let $B = B_i, B_{i+1}, \ldots, B_j$ 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 $\sigma_{i,i}(G) = [\delta(r(B)),\gamma(B)]$, the second $\sigma_{i+1,i_C}(G)$, the second $\sigma_{i_C+1,i_L}(G)$, and the second $\sigma_{i_L+1,j}(G)$, 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 $u \in V^{\mathrm{C}}_{\mathrm{cut}}$ (resp., $u \in V^{\mathrm{L}}_{\mathrm{cut}}$ and $u \in V^{\mathrm{R}}_{\mathrm{cut}}$). We denote these subsequences by $\sigma(B;G)$, $\sigma_{\mathrm{C}}(G(B);G)$, $\sigma_{\mathrm{L}}(G(B);G)$, and $\sigma_{\mathrm{R}}(G(B);G)$, respectively. Hence $\sigma(G(B);G) = [\sigma(B;G),\sigma_{\mathrm{C}}(G(B);G),\sigma_{\mathrm{L}}(G(B);G),\sigma_{\mathrm{R}}(G(B);G)]$.

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 $\overline{\sigma_{\mathrm{L}}}(G(B);G)$ (resp., $\overline{\sigma_{\mathrm{R}}}(G(B);G)$) denote the sequence obtained from $\sigma_{\mathrm{L}}(G(B);G)$ (resp., $\sigma_{\mathrm{R}}(G(B);G)$) by replacing $\gamma'(B')$ with $\overline{\gamma}(B')$ for all blocks B' such that $r(B') \in V'(B)$. Denote $\overline{\sigma_f}(G(B);G) = [\sigma(B;G),\sigma_{\mathrm{C}}(G(B);G), \overline{\sigma_{\mathrm{R}}}(G(B);G),\overline{\sigma_{\mathrm{L}}}(G(B);G)]$.

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

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

$$\sigma(G) \geq \sigma(G') \Leftrightarrow [\sigma_{\mathrm{L}}(G(B);G),\sigma_{\mathrm{R}}(G(B);G)] \geq [\overline{\sigma_{\mathrm{R}}}(G(B);G),\overline{\sigma_{\mathrm{L}}}(G(B);G)]. \tag{2}$$

For simplicity, let σ^{L} denote $\sigma^{\mathrm{L}}(G(B);G)$. Similarly for σ_{R}.

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

$$[\sigma_{\mathrm{L}},\sigma_{\mathrm{R}}] > [\overline{\sigma_{\mathrm{R}}},\overline{\sigma_{\mathrm{L}}}]$$

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

Assume $\sigma_{\mathrm{L}} > \overline{\sigma_{\mathrm{R}}}$. If $\sigma_{\mathrm{L}} \gg \overline{\sigma_{\mathrm{R}}}$, then we have $[\sigma_{\mathrm{L}}, \sigma_{\mathrm{R}}] > [\overline{\sigma_{\mathrm{R}}}, \overline{\sigma_{\mathrm{L}}}]$. We assume $\sigma_{\mathrm{L}} \sqsupset \overline{\sigma_{\mathrm{R}}}$. If $|\sigma_{\mathrm{L}}| = |\overline{\sigma_{\mathrm{R}}}|$, then we again obtain $[\sigma_{\mathrm{L}}, \sigma_{\mathrm{R}}] > [\overline{\sigma_{\mathrm{R}}}, \overline{\sigma_{\mathrm{L}}}]$. Assume that $|\sigma_{\mathrm{L}}| > |\overline{\sigma_{\mathrm{R}}}|$ holds. In this case, the first code $\gamma'(B_a)$ in $\overline{\sigma_{\mathrm{L}}}$ is compared with the $(|\sigma_{\mathrm{L}}|+1)$st code $\gamma'(B_b)$ in σ_{L}, and it suffices to show that $\gamma'(B_b) > \gamma'(B_a)$. Let B'_a (resp., B'_b) be the block such that $r(B_a) \in V'(B'_a)$ (resp., $r(B_b) \in V'(B'_b)$), and let $\gamma'(B_a) = (d(B'_a), \mathrm{side}(r(B_a)), \ell(r(B_a)), \gamma(B_a))$ and $\gamma'(B_b) = (d(B'_b), \mathrm{side}(r(B_b)), \ell(r(B_b)), \gamma(B_b))$. It holds $d(B'_b) \geq d(B)+1 = d(B'_a)$. If $d(B'_a) = d(B'_b) = d(B)+1$ holds, then we have $\gamma'(B_b) > \gamma'(B_a)$ by $\mathrm{side}(r(B_b)) = 2 > 1 = \mathrm{side}(r(B_a))$, 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 $B_i \in BS[v] = (B'_1, B'_2, \ldots, B'_p)$, 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, then it holds $\overline{\sigma_{\mathrm{R}}}(G(B); G) > \sigma_{\mathrm{L}}(G(B); G)$ by Lemma 3. Hence by the definition of left-side-heaviness, the embedding $G' = G/B^f$ obtained from G by flipping B 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 $B'_1, B'_2, \ldots, B'_q \in BS[v]$ in G lexicographically maximizes $[\gamma'(B'_1), \gamma'(B'_2), \ldots, \gamma'(B'_q)]$, and is unique, since either $\gamma'(B'_i) > \gamma'(B'_j)$ or $\gamma'(B'_j) > \gamma'(B'_i)$ whenever blocks B'_i and B'_j 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 $\overline{\sigma_f}(G(B); G)$. 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 $\mathcal{P}_{\mathcal{H}}(G)$ (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 $B^1, B^2, \ldots, B^p$ be the spine of G, let $G' = \mathcal{P}_{\mathcal{H}}(G)$, and $H' \in \mathcal{H}$ be the graph represented by G'. Then $\sigma(G')$ is obtained from $\sigma(G)$ by deleting the last code $\gamma'(B^p)$ or replacing $\gamma'(B^p) = (d(B^p), \mathrm{side}(r(B^p)), \ell(r(B^p)), \gamma(B^p))$ with $(d(B^p), \mathrm{side}(r(B^p)), \ell(r(B^p)), \gamma(\mathcal{P}_{\mathcal{B}}(B^p)))$. 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_k of B_i with $v = r(B_k)$, 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* $\mathrm{ps}(v, B_i)$ 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 $\mathrm{ps}(B_h, B_i) = \emptyset$ if $k = i$.

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

A left (resp., right) child-block B_a of a block B is called *opposing* with a right (resp., left) child-block B_b of B. Let $\gamma'(B) \simeq \gamma'(B')$ mean $\gamma'(B) = \overline{\gamma}'(B')$ if block B is opposing with B', and $\gamma'(B) = \gamma'(B')$

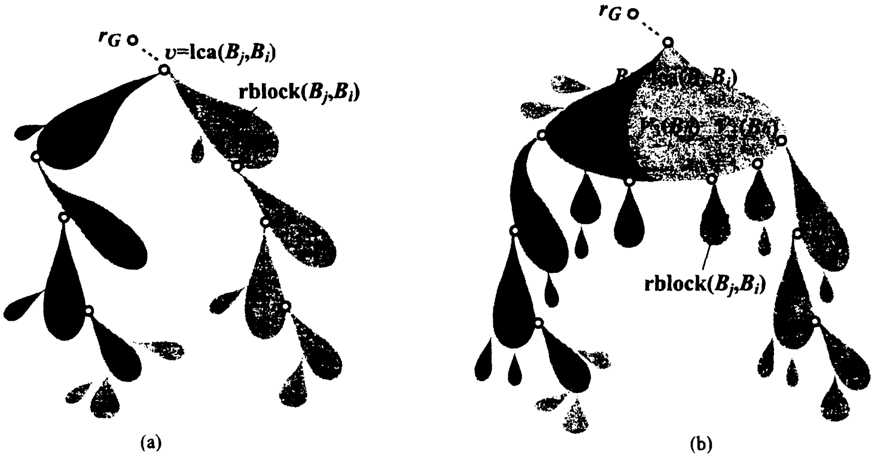

Figure 2: Two possible cases where a block B_j is pre-identical to a block B_i, (a) $\mathrm{lca}(B_i, B_j)$ is a vertex v; (b) $\mathrm{lca}(B_i, B_j)$ is a block B_h.

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

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

Note that $\mathrm{ps}(B_h, B_j) \simeq \mathrm{ps}(B_h, B_i)$ holds only when B_h is symmetric and the *initial* ancestor-block $B_{i'}$ of B_i (resp., $B_{j'}$ 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 $\mathrm{ps}(\mathrm{lca}(B_i, B_j), B_j) \simeq \mathrm{ps}(\mathrm{lca}(B_i, B_j), B_i)$.

If B_i has a left sibling B_j at $v = r(B_i)$, then B_j is pre-identical to B_i, where $\mathrm{ps}(v, B_j) = \mathrm{ps}(v, B_j) = \emptyset$. 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 $\mathrm{ps}(\mathrm{lca}(B_d, B_b), B_d) \simeq \mathrm{ps}(\mathrm{lca}(B_d, B_b), B_b)$. 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 $\mathrm{ps}(\mathrm{lca}(B_d, B_c), B_d) \simeq \mathrm{ps}(\mathrm{lca}(B_d, B_c), B_c)$. 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 $\mathcal{P}_{\mathcal{H}}(G)$.

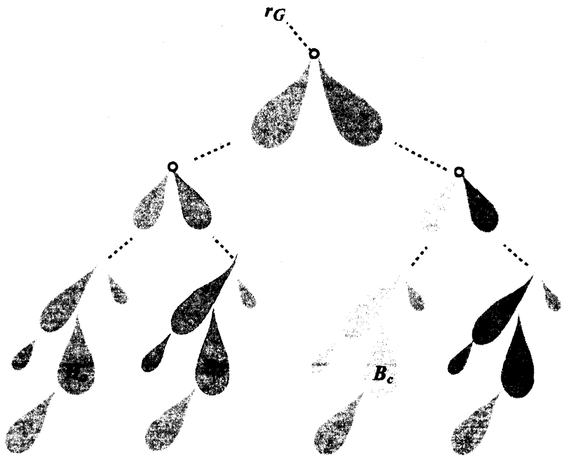

Figure 3: Illustration for two blocks B_j and B_k $(k < j < i)$ pre-identical to a block B_i.

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

Algorithm 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; 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 GEN(G).

Procedure 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 $B \in \mathcal{C}_{\mathcal{B}}(B^p)$. 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 EXPANDTIP: the task of extending the tip-block B^p of G to each of all children $B \in \mathcal{C}_{\mathcal{B}}(B^p)$.

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 $\tilde{B} \in \mathcal{B}$ 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 $\mathrm{key}(v) < \min\{\mathrm{key}(u) \mid V_{\mathrm{cut}}(B^i)\}$, where $\min\{\mathrm{key}(u) \mid V_{\mathrm{cut}}(B^p)\} = \infty$ for the tip-block B^p of G.

Lemma 7 *Let B_j and B_i ($j < i$) be blocks in the spine of a canonical embedding G. Assume that the child-embedding G'_i is obtained from G by appending a new seed block to a vertex $u \in V'(B^i)$. Then the child-embedding G'_j obtained from G by appending a seed block to any vertex $v \in V'(B^j)$ satisfying* $\mathrm{key}(v) < \min\{\mathrm{key}(u) \mid V_{\mathrm{cut}}(B^j)\}$ *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'_i 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 $\mathrm{key}(v) \leq \mathrm{endkey}^h$ 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 $\mathrm{rblock}(B_i, B_j)$ be the ancestor-block B_h of B_j with $r(B_h) = \mathrm{lca}(B_i, B_j)$ if $\mathrm{lca}(B_i, B_j)$ is a vertex; let $\mathrm{rblock}(B_i, B_j)$ be the first right child-block of block $\mathrm{lca}(B_i, B_j)$ 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^* be the block in the spine with $d(B^*) = d(B_l)$.*

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

(iii) *In the other case than (i)-(ii), B^h is given by B^* and $\mathrm{endkey}^h = \mathrm{key}(r(B_{j+1}))$ (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 $\mathrm{lca}(B_j, B_K) = B^* = B_l$ (see Fig. 4(a));

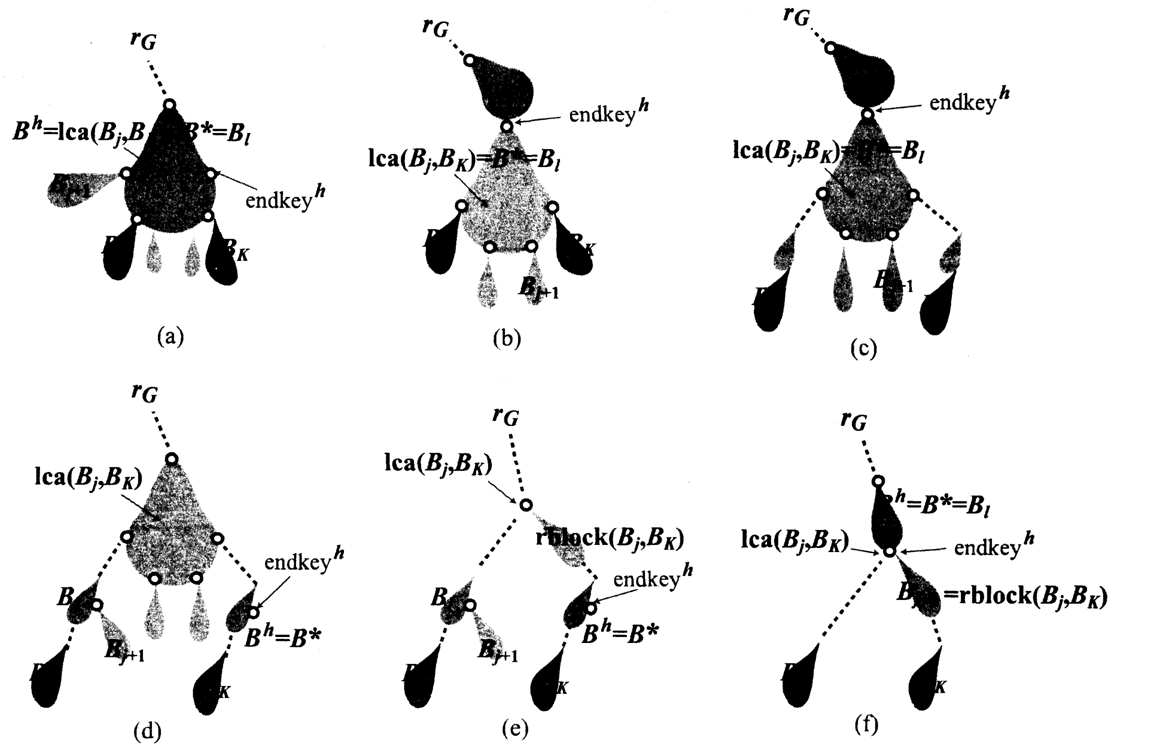

Figure 4: Illustration for the six subcases of the case where the tip-block $B_K = B^p$ has the competitor B_j with $\gamma'(B_j) \simeq \gamma'(B_K)$.

(b) B_{j+1} is the first right child-block of symmetric block $\mathrm{lca}(B_j, B_K) = B^* = B_l$, and B_j and B_K are right and left child-blocks of $\mathrm{lca}(B_j, B_K)$ (see Fig. 4(b));
(c) B_{j+1} is the first right child-block of symmetric block $\mathrm{lca}(B_j, B_K) = B^* = B_l$, and both B_j and B_K are not child-blocks of $\mathrm{lca}(B_j, B_K)$ (see Fig. 4(c));
(d) B_{j+1} is a descendant-block of a left child-block of symmetric block $\mathrm{lca}(B_j, B_K)$ (see Fig. 4(d));
(e) B_{j+1} is a descendant-block of a left child-block of vertex $\mathrm{lca}(B_j, B_K)$ (see Fig. 4(e)); and
(f) B_{j+1} is the child-block $\mathrm{rblock}(B_j, B_K)$ of vertex $\mathrm{lca}(B_j, B_K)$ (see Fig. 4(f)).

Let B^h and $\mathrm{endkey}^h = \mathrm{key}(r(B_{j+1}))$ be the block and the key value determined by the lemma. Then we see that the block $\mathrm{lca}(B_j, B_K)$ or $\mathrm{rblock}(B_j, B_K)$ 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 $\mathrm{key}(u) > \mathrm{endkey}^h$ 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 $\mathrm{key}(v) = \mathrm{endkey}^h$ 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 $B_l = B^h = \mathrm{lca}(B_j, B_K)$ remains left-side-heavy in G', we have $a < l$. Then the new tip-block B' has a pre-identical block B_t 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. ∎

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* $\mathrm{endkey}^h = \infty$.

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

We are ready to examine when the embedding G' obtained from G by extending the tip-block B^p to one of its child $B \in \mathcal{C}_{\mathcal{B}}(B^p)$ 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 $B \in \mathcal{C}_{\mathcal{B}}(B^p)$. 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 $\mathrm{lca}(B_j, B^p)$ is a block B_l, then we see that B_l is not left-side-heavy in G'. Otherwise if $\mathrm{lca}(B_j, B^p)$ is a vertex v, then there are two consecutive siblings $B_{j'}, B_{j''} \in BS[v]$ such that $B_{j'}$ and $B_{j''}$ are ancestor-blocks of B_j and B^p, indicating that $B_{j''}$ 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-sibling-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-sibling-heavy in G'. Then the left sibling $B_{k'} \in BS[v]$ of B_k at the root $v = r(B_h)$ 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 $(d(B_c), \mathrm{key}(r(B_c))) = (d(B^p), \mathrm{key}(r(B^p)))$ 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 $(d(B_b), \mathrm{key}(r(B_b))) = (d(B^p), \mathrm{key}(r(B^p)))$ (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, $(d(B_b), \mathrm{key}(r(B_b))) = (d(B_c), \mathrm{key}(r(B_c))) = (d(B^p), \mathrm{key}(r(B^p)))$ 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.

We 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 $(d(B_c), \mathrm{key}(r(B_c))) = (d(B^p), \mathrm{key}(r(B^p))$ (or $\mathrm{side}(r(B_c)) = 2$, $\mathrm{side}(r(B^p)) = 1$, and $(d(B_c), \ell(B_c)) = (d(B^p), \ell(B^p))$ if B_c and

B^p are child-blocks of B_k). By definition, B^p has the competitor B_b with $b \le c$. 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 $(d(B_b), \mathrm{key}(r(B_b))) = (d(B^p), \mathrm{key}(r(B^p)))$. By Lemma 6, it holds $\gamma'(B_c) \ge \gamma'(B_b) \ge \gamma'(B^p)$. Again this and $\gamma(B) > \gamma(B_c) \ge \gamma(B^p)$ 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 $B_{\min} := \tilde{B}$ and $B_{\max} := C(B_K)$ (let $B_{\max} := \infty$ if $C(B_K) := \emptyset$) ;
  while B :=NextMinChild$(B_K, B_{\min}, B_{\max}) \ne \emptyset$ and $|V(G)| + |V'(B)| \le n$ **do**
    B :=NextMinChild$(B_K, B_{\min}, B_{\max})$;
    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');
    $B_{\min} := B$
  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 := 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$) \ne \emptyset$ **do**
    $(v, \mathrm{key}(v))$:=NextVertex$(B^i$, currentkey);
    Create a new block B which is equivalent to seed block $\tilde{B}$;
    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 := key(v);
    if currentkey = endkey^i **then** currentkey := ∞
      /* 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 $B \in \mathcal{B}$ is stored in a linked list $LIST(B)$ in the decreasing order with respect to their levels ℓ, and that the following procedure NextVertex of reporting the current vertex in $LIST(B)$ is available.

Procedure NextVertex(B, κ)

Input: A block B and a key value $\kappa \in (\{1,2,3\} \times \mathcal{Z}) \cup \{-\infty, \infty\}$, where $\mathcal{Z}$ denotes the set of integers.
Output: The vertex name u and $\mathrm{key}(u) = (\mathrm{side}(u), \ell(u))$ of the vertex next to the vertex $v \in V(B)$ with $\mathrm{key}(v) = \kappa$ in a list $LIST(B)$ of vertices to which a block can be attached, where we choose such a vertex u from $V_3(B)$, $V_2(B)$, $V_1(B)$ in this order and the first such vertex is chosen when $\kappa = -\infty$; return $\emptyset$ if no such a nonroot vertex v of B exists or $\kappa = \infty$.

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

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

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

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 $\mathrm{lca}(B_i, B_j)$ and $\mathrm{rblock}(B_i, B_j)$:

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

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

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

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

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

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

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

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

Proof. If B_i has a left sibling at $v = r(B_i)$, then B_i 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_i is the first right child-block of its parent-block B_l, then B_l has a left child-block and thereby B_i has a competitor.

(i) Assume that there is no block pre-identical to B_i. We show that no competitor is given to B_i in Case-C1 and C2. Since B_j 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 $\mathrm{lca}(B_i, B_j) = \mathrm{lca}(B_{i-1}, B_{j-1})$ 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 $\mathrm{ps}(v, B_{j-1}) = \mathrm{ps}(v, B_{i-1})$. Since $\gamma'(B_{j-1}) = \gamma'(B_{i-1})$ holds, it holds $\mathrm{ps}(v, B_j) = [\mathrm{ps}(v, B_{j-1}), \gamma'(B_{j-1})] = [\mathrm{ps}(v, B_{i-1}),$

$\gamma'(B_{i-1})] = \mathrm{ps}(v, B_i)$. 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 $BS[v]$ at $v = r(B_i)$, then no competitor is assigned to B_i in Case-C1, which implies that B_t is assigned to B_i as the competitor of B_i 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_i and B_t are the first left- and right-blocks of a block analogously.

Assume that B_i and B_t do not satisfy each of conditions (a) and (b) in Case-C2. In this case, the preceding block B_{t-1} of B_t is pre-identical to the preceding block B_{i-1} of B_i. Hence if the competitor of B_{i-1} is B_{t-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 $\gamma'(B_{t-1}) \simeq \gamma'(B_{i-1})$, 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. ∎

Whether $\mathrm{lca}(B_i, B_j) = \mathrm{lca}(B_{i-1}, B_{j-1})$ or not can be tested using $\mathrm{lca}(B_{i-1}, B_{j-1})$ and $\mathrm{rblock}(B_{i-1}, B_{j-1})$ as follows: $\mathrm{lca}(B_i, B_j) = \mathrm{lca}(B_{i-1}, B_{j-1})$ if and only if $j < h$ and $d(B_h) > d(B_i)$ for $B_h = \mathrm{rblock}(B_{i-1}, B_{j-1})$. Hence we can determine the competitor $C(B)$ of a new block B according to Cases-C1 and C2 in $O(1)$ time.

Finally we consider the entire algorithm GENERATE. For the correctness of GENERATE, we only need to show that, when 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 GEN(G), task AppendSeed is executed only when $|V(G)| + |V'(\tilde{B})| \le n$. We see that, if $|V(G)| + |V'(\tilde{B})| > n$, 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 (S5) of γ. Similarly, 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^p to any other unseen children $B' \in \mathcal{C}_{\mathcal{B}}$, because $\gamma(B') > \gamma(B)$ holds by the listing order of NextMinChild and thereby $|V(B')| \ge |V(B)| > n$ holds by the monotonicity (S4) of γ.

It is not difficult to implement 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 NextVertex and NextMinChild, where Δ denotes the maximum size between two consecutive outputs. Let $T(n)$ and $S(n)$ denote the time and space complexities of procedures NextVertex and NextMinChild. Then we see that all rooted graphs in $\mathcal{H}$ can be generated by 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 $\mathcal{B}$ be a class of blocks which admits signature γ monotone with respect to the number of vertices. Then all canonical embeddings of rooted graphs in a class $\mathcal{H}$ over $\mathcal{B}$ 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 reflectional 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 NextVertex and 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.

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