1 Pseudo-codes for Graph Search Algorithm

1.1 Enumeration Algorithm of Fringe-Trees via Sequence Representations

For an acyclic chemical graph $G = (H, \alpha, \beta)$ on n vertices, let $V(H) = \{v_1, v_2, \ldots, v_n\}$ be such that $\deg_H(v_n) = 1$. We say that G is rooted at v_1. Let pred : $[2, n] \to [1, n-1]$ be a bijection such that for $k \in [2, n]$, $v_k v_{\mathrm{pred}(k)} \in E(H)$. We call the alternating sequence $S \triangleq (\alpha(v_1), \beta(v_{\mathrm{pred}(2)} v_2), \alpha(v_2),$ $\ldots, \beta(v_{\mathrm{pred}(n)} v_n), \alpha(v_n))$ the *sequence representation* of G.

Algorithm SeqMap$(\Lambda, \boldsymbol{x}^*, \delta)$
Input: A set Λ of chemical elements,
  a vector $\boldsymbol{x}^* = (\boldsymbol{x}^*_{\mathrm{co}}, \boldsymbol{x}^*_{\mathrm{in}}, \boldsymbol{x}^*_{\mathrm{ex}}, b)$ with $\boldsymbol{x}^*_{\mathrm{co}} \in \mathbb{Z}^{\Lambda^{\mathrm{co}}}$, $\boldsymbol{x}^*_{\mathtt{t}} \in \mathbb{Z}^{\Lambda^{\mathtt{t}}}$, $\mathtt{t} \in \{\mathrm{in}, \mathrm{ex}\}$, $b \in \mathbb{Z}_+$ and
  an integer δ.
Output: The set of sequence representations of all acyclic graphs G and
  their frequency vectors $\boldsymbol{w} = (\boldsymbol{w}_{\mathrm{co}}, \boldsymbol{w}_{\mathrm{in}}, \boldsymbol{w}_{\mathrm{ex}}, 0)$ such that $\boldsymbol{w} \le \boldsymbol{x}^*$, degree of root in G is 1, and
  G has $\delta + 1$ vertices,
  where the set of these sequences is stored in a trie.
for each $t = \mathtt{a} \in \Lambda$ **do**
  $\mathrm{Cld}_t := \mathrm{Leaf}_t := \emptyset$;
  for each $\mathtt{b} \in \Lambda$ and $m \in [1, 3]$ such that $\mathrm{val}(\mathtt{a}) \ge m, \mathrm{val}(\mathtt{b}) \ge m$ **do**
    Let $S := (\mathtt{a}, m, \mathtt{b})$; /* Sequence representation of a tree with two vertices */
    if Trie$(m, \mathtt{b}, S, \delta - 1)$ returns a node v_γ and
     a leaf set Leaf_γ **then**
      $\mathrm{Leaf}_t := \mathrm{Leaf}_t \cup \mathrm{Leaf}_\gamma$; $\mathrm{Cld}_t := \mathrm{Cld}_t \cup \{v_\gamma\}$
    endif
  endfor;
  if $\mathrm{Cld}_t \ne \emptyset$ **then**
    Create a new node u_t as the parent of nodes in Cld_t;
    Sort the leaves $u \in \mathrm{Leaf}_t$ in lexicographically descending order
     with respect to $\mathrm{key}(u) = (S_u, \mathtt{a}_u, h_u)$;
    Partition Leaf_t into subsets $\mathrm{Leaf}_t^{(i)}$, $i = 1, 2, \ldots, m_t$ so that $\mathrm{key}(u) = \mathrm{key}(u')$
      if and only if $u, u' \in \mathrm{Leaf}_t^{(i)}$ for some i;
    For each $i = 1, 2, \ldots, m_t$, create a new node $u_{t,i}$ (called a superleaf) to the leaves in $\mathrm{Leaf}_t^{(i)}$
      and define $\mathrm{key}(u_{t,i})$ to be $\mathrm{key}(u) = (S_u, \mathtt{a}_u, h_u)$ for a leaf $u \in \mathrm{Leaf}_t^{(i)}$
  endif;
  Set $\mathrm{S}^{(\delta)}[\boldsymbol{x}^*, t]$ to be the set of sequences $S = \mathrm{key}_1(u_{t,i})$ for all superleaves $u_{t,i}$
endfor;
Output $\{\mathrm{S}^{(\delta)}[\boldsymbol{x}^*, t] \mid t \in \Lambda\}$ as the required set of sequence representation of acyclic graphs, and
  for each $S \in \{\mathrm{S}^{(\delta)}[\boldsymbol{x}^*, t] \mid t \in \Lambda\}$, the frequency vector of the graph

of which the sequence representation is S.

Recursive Procedure $\textsc{Trie}(h, \mathtt{a}, S, \delta)$
Input: A set Λ of chemical elements,
a vector $\boldsymbol{x}^* = (\boldsymbol{x}^*_{\mathrm{co}}, \boldsymbol{x}^*_{\mathrm{in}}, \boldsymbol{x}^*_{\mathrm{ex}}, b)$ with $\boldsymbol{x}^*_{\mathrm{co}} \in \mathbb{Z}^{\Lambda^{\mathrm{co}}}$, $\boldsymbol{x}^*_{\mathtt{t}} \in \mathbb{Z}^{\Lambda^{\mathtt{t}}}$, $\mathtt{t} \in \{\mathrm{in}, \mathrm{ex}\}$,
$b \in \mathbb{Z}_+$ (global constants),
an integer $h \in [1, 3]$, an element $\mathtt{a} \in \Lambda$,
a sequence representation S, and
an integer $\delta \geq 0$.
Output: The set of sequence representation of graphs G rooted at atom $\mathtt{a}$, with $\delta + 1$ vertices
that can be extended from S, and
frequency vector $\boldsymbol{w}$ of G when $\delta = 0$ and $\boldsymbol{w} \leq \boldsymbol{x}^*$,
where the set of these sequences is stored in a trie.
A trie that stores all sequences of length δ from atom $\mathtt{a}$
with a j-bond ($j \in [1, \mathrm{val}(\mathtt{a}) - h]$);
if $\delta = 0$ **then**
  if the frequency vector of the graph with sequence representation S is at most $\boldsymbol{x}^*$
   where we do not consider the configuration of the edge with root as an end vertex **then**
    Create a new leaf node u with $\mathrm{key}(u) = (S, \mathtt{a}, h)$, return u and a leaf set $\mathrm{Leaf} := \{u\}$
  end if
else
  $\mathrm{Cld} := \mathrm{Leaf} := \emptyset$;
  for each $\mathtt{b} \in \Lambda$ and $m \in [1, 3]$ with $\mathrm{val}(\mathtt{a}) \geq m + h, \mathrm{val}(\mathtt{b}) \geq m$ **do**
    if $\textsc{Trie}(m + h, \mathtt{b}, (S, m, \mathtt{b}), \delta - 1)$ returns a node v and
     a leaf set Leaf_v **then**
      $\mathrm{Cld} := \mathrm{Cld} \cup \{v\}$; $\mathrm{Leaf} := \mathrm{Leaf} \cup \mathrm{Leaf}_v$
    endif
  endfor;
  if $\mathrm{Cld} = \emptyset$ **then**
    Return `empty`
  endif
endif.

1.2 Generating All Fringe Trees

We enumerate all possible 2-fringe-trees rooted at vertices with label $\mathtt{a}$ in Λ, under a given resource vector $\boldsymbol{x}^* = (\boldsymbol{x}^*_{\mathrm{co}}, \boldsymbol{x}^*_{\mathrm{in}}, \boldsymbol{x}^*_{\mathrm{ex}}, b)$.

FringeTreeWeightVectors($\mathtt{a}$)

Input: A vector $\boldsymbol{x}^* = (\boldsymbol{x}^*_{\rm co}, \boldsymbol{x}^*_{\rm in}, \boldsymbol{x}^*_{\rm ex}, b)$ with $\boldsymbol{x}^*_{\rm co} \in \mathbb{Z}^{\Lambda^{\rm co}}$, $\boldsymbol{x}^*_{\mathtt{t}} \in \mathbb{Z}^{\Lambda^{\mathtt{t}}}$, $\mathtt{t} \in \{\rm in, ex\}$,
two non-negative integers b and $h \leq 2 (= \rho)$, an element $\mathtt{a} \in \Lambda$ and an integer $g \geq 1$.

Output: The sets $\mathrm{W}^{(0)}_{\rm end}(\mathtt{a}, d, m; \boldsymbol{x}^*)$ (resp., $\mathrm{W}^{(0)}_{\rm inl}(\mathtt{a}, d, m; \boldsymbol{x}^*)$,
$\mathrm{W}^{(0)}_{\rm co+2}(\mathtt{a}, d, m, h; \boldsymbol{x}^*)$ and $\mathrm{W}^{(0)}_{\rm co+3}(\mathtt{a}, d, m, h; \boldsymbol{x}^*)$)
$d \in [1, \mathrm{val}(\mathtt{a}) - 1]$ (resp., $d \in [0, \mathrm{val}(\mathtt{a}) - 2]$ and $d \in [0, \mathrm{val}(\mathtt{a}) - 3]$) and
$m \in [d, \mathrm{val}(\mathtt{a}) - 1]$ (resp., $m \in [d, \mathrm{val}(\mathtt{a}) - 2]$ and $m \in [d, \mathrm{val}(\mathtt{a}) - 3]$)
and for each vector $\boldsymbol{w}$ in these sets, a set $\mathcal{T}_{\boldsymbol{w}}$ of sample trees $T_{\boldsymbol{w}}$ of size at most g and
the number $n_{\boldsymbol{w}}$ of all sample trees.

Step 1: Enumerate all fringe-trees T rooted at vertex v_r such that
$\alpha(v_r) = \mathtt{a}$, the height is 2, (resp., at most 2)
the degree $d_{\rm root}$ of v_r is 1 (i.e., v_r has exactly one child v_c) with
$\boldsymbol{f}(\gamma^{\rm ex}) \leq \boldsymbol{x}^*_{\rm ex}$
/* Using recursive algorithm SeqMap to enumerate these */
Let $\mathcal{T} = \{(T_i, k_i, d_i, \boldsymbol{w}^i_{\rm co}, \boldsymbol{w}^i_{\rm in}, \boldsymbol{w}^i_{\rm ex}) \mid i = 1, 2, \ldots, q\}$ denote the resulting set of fringe-trees,
where T_i denotes the i-th tree (say, generated as the i-th solution),
k_i denotes the multiplicity of edge $v_r v_c$,
d_i denotes the degree of child v_c, $\boldsymbol{w}^i_{\rm in} = \boldsymbol{f}_{\rm in}(T_i)$, and
$\boldsymbol{w}^i_{\rm ex} = \boldsymbol{f}_{\rm ex}(T_i) - \mathbf{1}_\gamma$ for $\gamma = (\mathtt{a}1, \mathtt{b}d_c, k_i)$ and $\alpha(v_c) = \mathtt{b}$;

Step 2: Enumerate all fringe-trees T with $d_{\rm root} \in [1, 2, 3]$ as follows:
$\mathrm{W}[\mathtt{a}, d, m] := \emptyset$ for $d \in [1, \mathrm{val}(\mathtt{a}) - 1]$, $m \in [d, \mathrm{val}(a) - d]$;
Let $\mathrm{dg}^+ := 1$ (resp., $\mathrm{dg}^+ := 2$, and $\mathrm{dg}^+ := 3$);
for each $i \in [1, q]$ **do**
 if $|V(T_i)| \leq 4$, $\boldsymbol{w}^i_{\rm ex} + \mathbf{1}_{\gamma(i)} \leq \boldsymbol{x}^*_{\rm ex}$ holds for $\gamma(i) := (\mathtt{a}\{\mathrm{dg}^+ + 1\}, \mathtt{b}d_i, k_i)$ **then**
  /* Also test if the height of the tree T_i is exactly equal to 2 (resp., h) while
   constructing $\mathrm{W}^{(0)}_{\rm end}(a, d, m; \boldsymbol{x}^*)$ (resp., $\mathrm{W}^{(0)}_{\rm co+2}(\mathtt{a}, d, m, h; \boldsymbol{x}^*)$ and $\mathrm{W}^{(0)}_{\rm co+3}(\mathtt{a}, d, m, h; \boldsymbol{x}^*)$) */
  Let $\boldsymbol{w} := (\boldsymbol{w}^i_{\rm co}, \boldsymbol{w}^i_{\rm in}, \boldsymbol{w}^i_{\rm ex} + \mathbf{1}_{\gamma(i)}, 0)$;
  if $\boldsymbol{w} \in \mathrm{W}[\mathtt{a}, 1, k_i]$ **then** $n_{\boldsymbol{w}} := n_{\boldsymbol{w}} + 1$
   if $|\mathcal{T}_{\boldsymbol{w}}| < g$ **then** $\mathcal{T}_{\boldsymbol{w}} := \mathcal{T}_{\boldsymbol{w}} \cup \{T_i\}$
  else $\mathrm{W}[\mathtt{a}, 1, k_i] := \mathrm{W}[\mathtt{a}, 1, k_i] \cup \{\boldsymbol{w}\}$; $\mathcal{T}_{\boldsymbol{w}} := \{T_i\}$; $n_{\boldsymbol{w}} := 1$ **endif**
 endif;
 for each $j \in [i, q]$ **do**
  if $k_i + k_j \leq \mathrm{val}(\mathtt{a}) - \mathrm{dg}^+$ **then**
   for each $h \in [j, q]$ **do**
    Let $\mathtt{b}_i, \mathtt{b}_j, \mathtt{b}_k$ be the labels of the child of the roots of T_i, T_j, T_k, respectively;
    $\gamma(i) := (\mathtt{a}\{\mathrm{dg}^+ + 3\}, \mathtt{b}_i d_i, k_i)$; $\gamma(j) := (\mathtt{a}\{\mathrm{dg}^+ + 3\}, \mathtt{b}_j d_j, k_j)$; $\gamma(i) := (\mathtt{a}\{\mathrm{dg}^+ + 3\}, \mathtt{b}_h d_h, k_h)$;
    if $k_i + k_j + k_h \leq \mathrm{val}(\mathtt{a}) - \mathrm{dg}^+$ (i.e., $k_i = k_j = k_h = 1$ and $\mathrm{val}(\mathtt{a}) = 4$),
     $\boldsymbol{w}^i_{\rm ex} + \boldsymbol{w}^j_{\rm ex} + \boldsymbol{w}^h_{\rm ex} + \mathbf{1}_{\gamma(i)} + \mathbf{1}_{\gamma(j)} + \mathbf{1}_{\gamma(h)} \leq \boldsymbol{x}^*_{\rm ex}$
     and $|V(T_i)| + |V(T_j)| + |V(T_h)| - 2 \leq 8$ **then**
      /* Also test if the height of at least one tree T_i, T_j, T_h is exactly equal to 2 while

constructing $\mathrm{W}^{(0)}_{\mathrm{end}}(a, d, m; \boldsymbol{x}^*)$ */
$\boldsymbol{w} := (\boldsymbol{w}^i_{\mathrm{co}} + \boldsymbol{w}^j_{\mathrm{co}} + \boldsymbol{w}^h_{\mathrm{co}}, \boldsymbol{w}^i_{\mathrm{in}} + \boldsymbol{w}^j_{\mathrm{in}} + \boldsymbol{w}^h_{\mathrm{in}}, \boldsymbol{w}^i_{\mathrm{ex}} + \boldsymbol{w}^j_{\mathrm{ex}} + \boldsymbol{w}^h_{\mathrm{ex}} + \mathbf{1}_{\gamma(i)} + \mathbf{1}_{\gamma(j)} + \mathbf{1}_{\gamma(h)}, 0)$;
Let T be the tree obtained by identifying the roots of T_i, T_j, and T_h;
$m := k_i + k_j + k_h$;
if $\boldsymbol{w} \in \mathrm{W}[\mathtt{a}, 3, m]$ **then** $n_{\boldsymbol{w}} := n_{\boldsymbol{w}} + 1$
if $|\mathcal{T}_{\boldsymbol{w}}| < g$ **then** $\mathcal{T}_{\boldsymbol{w}} := \mathcal{T}_{\boldsymbol{w}} \cup \{T\}$
else
$\mathrm{W}[\mathtt{a}, 3, m] := \mathrm{W}[\mathtt{a}, 3, m] \cup \{\boldsymbol{w}\}$; $\mathcal{T}_{\boldsymbol{w}} := \{T\}$; $n_{\boldsymbol{w}} := 1$;
endif
endif
endfor;
$\gamma(i) := (\mathtt{a}\{\mathrm{dg}^+ + 2\}, \mathtt{b}_i d_i, k_i)$; $\gamma(j) := (\mathtt{a}(\mathrm{dg}^+ + 2), \mathtt{b}_j d_j, k_j)$;
if $|V(T_i)| + |V(T_j)| - 1 \le 6$,
$\boldsymbol{w}^i_{\mathrm{ex}} + \boldsymbol{w}^j_{\mathrm{ex}} + \mathbf{1}_{\gamma(i)} + \mathbf{1}_{\gamma(j)} \le \boldsymbol{x}^*_{\mathrm{ex}}$ **then**
/* Also test if the height of at least one tree T_i, T_j is exactly equal to 2 (resp., h) while constructing $\mathrm{W}^{(0)}_{\mathrm{end}}(a, d, m; \boldsymbol{x}^*)$ (resp., $\mathrm{W}^{(0)}_{\mathrm{co+2}}(\mathtt{a}, d, m, h; \boldsymbol{x}^*)$) */
$\boldsymbol{w} := (\boldsymbol{w}^i_{\mathrm{co}} + \boldsymbol{w}^j_{\mathrm{co}}, \boldsymbol{w}^i_{\mathrm{in}} + \boldsymbol{w}^j_{\mathrm{in}}, \boldsymbol{w}^i_{\mathrm{ex}} + \boldsymbol{w}^j_{\mathrm{ex}} + \mathbf{1}_{\gamma(i)} + \mathbf{1}_{\gamma(j)}, 0)$;
Let T be the tree obtained by identifying the roots of T_i and T_j;
$m := k_i + k_j$;
if $w \in \mathrm{W}[\mathtt{a}, 2, m]$ **then** $n_{\boldsymbol{w}} := n_{\boldsymbol{w}} + 1$
if $|\mathcal{T}_{\boldsymbol{w}}| < g$ **then** $\mathcal{T}_{\boldsymbol{w}} := \mathcal{T}_{\boldsymbol{w}} \cup \{T\}$
else
$\mathrm{W}[\mathtt{a}, 2, m] := \mathrm{W}[\mathtt{a}, 2, m] \cup \{\boldsymbol{w}\}$; $\mathcal{T}_{\boldsymbol{w}} := \{T\}$; $n_{\boldsymbol{w}} := 1$
endif
endif
endif
endfor
endfor;
/* It remains to calculate the set $\mathrm{W}^{(0)}_{\mathrm{inl}}(\mathtt{a}, 0, 0; \boldsymbol{x}^*)$, $\mathrm{W}^{(0)}_{\mathrm{co+2}}(\mathtt{a}, 0, 0, h; \boldsymbol{x}^*)$ and $\mathrm{W}^{(0)}_{\mathrm{co+3}}(\mathtt{a}, 0, 0, h; \boldsymbol{x}^*)$ */
Let T be a singleton vertex labeled $\mathtt{a}$;
$\mathrm{W}[\mathtt{a}, 0, 0] := \{\boldsymbol{w} = (\mathbf{0}, \mathbf{0}, \mathbf{0}, 0)\}$; $\mathcal{T}_{\boldsymbol{w}} := \{T\}$; $n_{\boldsymbol{w}} := 1$;
Output $\mathrm{W}[\mathtt{a}, d, m]$ as $\mathrm{W}^{(0)}_{\mathrm{end}}(\mathtt{a}, d, m; \boldsymbol{x}^*)$ (resp., $\mathrm{W}^{(0)}_{\mathrm{inl}}(\mathtt{a}, d, m; \boldsymbol{x}^*)$, $\mathrm{W}^{(0)}_{\mathrm{co+2}}(\mathtt{a}, d, m, h; \boldsymbol{x}^*)$ and $\mathrm{W}^{(0)}_{\mathrm{co+3}}(\mathtt{a}, d, m, h; \boldsymbol{x}^*)$), for each $\boldsymbol{w} \in \mathrm{W}[\mathtt{a}, d, m]$, $\mathcal{T}_{\boldsymbol{w}}$, and $n_{\boldsymbol{w}}$.

1.3 Computing Frequency Vectors of End-Subtrees

For an integer $h \ge 1$, element $\mathtt{a} \in \Lambda$, integers $d \in [1, \mathrm{val}(\mathtt{a}) - 1]$, and $m \in [d, \mathrm{val}(\mathtt{a}) - 1]$ we give a procedure to compute the set $\mathrm{W}^{(h)}_{\mathrm{end}}(\mathtt{a}, d, m; \boldsymbol{x}^*)$.

ComputeEndSubtreeOne$(\mathtt{a}, d, m, h)$

Input: Element $\mathtt{a} \in \Lambda$, integer $d \in [1, \mathrm{val}(a) - 1]$, $m \in [d, \mathrm{val}(a) - 1]$, $h \ge 1$.
/* Global data: A vector $\boldsymbol{x}^* = (\boldsymbol{x}^*_{\mathrm{co}}, \boldsymbol{x}^*_{\mathrm{in}}, \boldsymbol{x}^*_{\mathrm{ex}}, b)$ with $\boldsymbol{x}^*_{\mathrm{co}} \in \mathbb{Z}^{\Lambda^{\mathrm{co}}}$, $\boldsymbol{x}^*_{\mathtt{t}} \in \mathbb{Z}^{\Lambda^{\mathtt{t}}}$, $\mathtt{t} \in \{\mathrm{in}, \mathrm{ex}\}$,

a non-negative integer b, the collection
$\mathcal{W}^{(0)}_{\rm inl}$ vector sets $\mathrm{W}^{(0)}_{\rm inl}(\mathtt{a}, d-1, m_{\mathtt{a}}; \boldsymbol{x}^*)$, $m_{\mathtt{a}} \in [d-1, \mathrm{val}(\mathtt{a})-2]$
$\mathcal{W}^{(h-1)}_{\rm end}$ of vector sets $\mathrm{W}^{(h-1)}_{\rm end}(\mathtt{a}_1, d_1, m_1; \boldsymbol{x}^*)$, $\mathtt{a}_1 \in \Lambda$, $d_1 \in [1, \mathrm{val}(\mathtt{a}_1)-1]$,
$m_1 \in [d_1, \mathrm{val}(\mathtt{a}_1)-1]$, and integer $g \geq 1$ and
for each vector w in these sets, a set $\mathcal{T}_{\boldsymbol{w}}$ of sample trees $T_{\boldsymbol{w}}$ of size at most g and
the number $n_{\boldsymbol{w}}$ of samples trees
with vector $\boldsymbol{w}$. */

Output: The set $\mathrm{W}^{(h)}_{\rm end}(\mathtt{a}, d, m; \boldsymbol{x}^*)$, where we store each vector $\boldsymbol{w} \in \mathrm{W}^{(h)}_{\rm end}(\mathtt{a}, d, m; \boldsymbol{x}^*)$,
a set $\mathcal{T}_{\boldsymbol{w}}$ of sample trees $T_{\boldsymbol{w}}$ of size at most g and number $n_{\boldsymbol{w}}$ of trees with vector $\boldsymbol{w}$ in a trie.

$\mathrm{W} := \emptyset$;
for each triplet $(\mathtt{b}, d_{\mathtt{b}}, m_{\mathtt{b}})$ **do**
  for each triplet $(\mathtt{a}, d-1, m_{\mathtt{a}})$ **do**
    for each $\boldsymbol{w}^{\mathtt{b}} = (\boldsymbol{w}^{\mathtt{b}}_{\rm co}, \boldsymbol{w}^{\mathtt{b}}_{\rm in}, \boldsymbol{w}^{\mathtt{b}}_{\rm ex}, 0) \in \mathrm{W}^{(h-1)}_{\rm end}(\mathtt{b}, d_{\mathtt{b}}, m_{\mathtt{b}}; \boldsymbol{x}^*)$ **do**
      for each $m' \in [1, 3]$ such that
        - $\gamma^{\rm in} = (\mathtt{a}\{d+1\}, \mathtt{b}\{d_{\mathtt{b}}+1\}, m') \in \Gamma^{\rm in}$ and
        - $m_{\mathtt{a}} + m' = m, m_{\mathtt{a}} + m' + 1 \leq \mathrm{val}(\mathtt{a})$ and $m' + m_{\mathtt{b}} \leq \mathrm{val}(\mathtt{b})$ **do**
        for each $\boldsymbol{w}^{\mathtt{a}} = (\boldsymbol{w}^{\mathtt{a}}_{\rm co}, \boldsymbol{w}^{\mathtt{a}}_{\rm in}, \boldsymbol{w}^{\mathtt{a}}_{\rm ex}, 0) \in \mathrm{W}^{(0)}_{\rm inl}(\mathtt{a}, d-1, m_{\mathtt{a}}; \boldsymbol{x}^*)$ **do**
          $\boldsymbol{w}_{\rm in} := \boldsymbol{w}^{\mathtt{a}}_{\rm in} + \boldsymbol{w}^{\mathtt{b}}_{\rm in} + \mathbf{1}_{\gamma^{\rm in}}$;
          $\boldsymbol{w}_{\rm ex} := \boldsymbol{w}^{\mathtt{a}}_{\rm ex} + \boldsymbol{w}^{\mathtt{b}}_{\rm ex}$; $\boldsymbol{w} := (\boldsymbol{w}_{\rm co}, \boldsymbol{w}_{\rm in}, \boldsymbol{w}_{\rm ex}, 0)$;
          if $\boldsymbol{w} \leq \boldsymbol{x}^*$ **then**
            if $\boldsymbol{w} \in \mathrm{W}$ **then** $n_{\boldsymbol{w}} = n_{\boldsymbol{w}} + n_{\boldsymbol{w}^{\mathtt{a}}} \cdot n_{\boldsymbol{w}^{\mathtt{b}}}$
            else
              $\mathrm{W} := \mathrm{W} \cup \{\boldsymbol{w}\}$; $\mathcal{T}_{\boldsymbol{w}} := \emptyset$; $n_{\boldsymbol{w}} := n_{\boldsymbol{w}^{\mathtt{a}}} \cdot n_{\boldsymbol{w}^{\mathtt{b}}}$
            end if
            if $\boldsymbol{w} \in \mathrm{W}$ **then**
              for each $T_{\boldsymbol{w}^{\mathtt{a}}} \in \mathcal{T}_{\boldsymbol{w}^{\mathtt{a}}}$ and $T_{\boldsymbol{w}^{\mathtt{b}}} \in \mathcal{T}_{\boldsymbol{w}^{\mathtt{b}}}$ **do**
                Let T be the tree obtained by joining the roots of $T_{\boldsymbol{w}^{\mathtt{a}}}$ and $T_{\boldsymbol{w}^{\mathtt{b}}}$
                  by an edge of multiplicity m';
                if $|\mathcal{T}_{\boldsymbol{w}}| < g$ **then** $\mathcal{T}_{\boldsymbol{w}} := \mathcal{T}_{\boldsymbol{w}} \cup \{T\}$
              end for
            end if
          end if
        end for
      end for
    end for
  end for
end for;
Output W as $\mathrm{W}^{(h)}_{\rm end}(\mathtt{a}, d, m; \boldsymbol{x}^*)$, and for each $\boldsymbol{w} \in \mathrm{W}$, $\mathcal{T}_{\boldsymbol{w}}$ and $n_{\boldsymbol{w}}$.

1.4 Computing Frequency Vectors of Internal Core-Subtrees

For integer $h \geq 0$, $\Delta \in [2, 3]$, elements $\mathtt{a}, \mathtt{a}' \in \Lambda$, integers $d_{\mathtt{a}} \in [0, \mathrm{val}(\mathtt{a}) - \Delta - 1]$, $m_{\mathtt{a}} \in [d_{\mathtt{a}}, \mathrm{val}(\mathtt{a}) - \Delta - 1]$, $d_{\mathtt{a}'} \in [1, \mathrm{val}(\mathtt{a}') - 1]$, $m_{\mathtt{a}'} \in [d_{\mathtt{a}'}, \mathrm{val}(\mathtt{a}') - 1]$, we define the set $\mathrm{W}^{(0)}_{\mathrm{co}+(\Delta+1)}(\mathtt{a}, d_{\mathtt{a}}, m_{\mathtt{a}}, \mathtt{a}', d_{\mathtt{a}'}, m_{\mathtt{a}'}, h; \boldsymbol{x}^*)$ such that for $h = 0$, $\mathrm{W}^{(0)}_{\mathrm{co}+(\Delta+1)}(\mathtt{a}, d_{\mathtt{a}}, m_{\mathtt{a}}, \mathtt{a}', d_{\mathtt{a}'}, m_{\mathtt{a}'}, h; \boldsymbol{x}^*) \triangleq \mathrm{W}^{(0)}_{\mathrm{co}+(\Delta+1)}(\mathtt{a}, d_{\mathtt{a}}, m_{\mathtt{a}}, p; \boldsymbol{x}^*)$ for some $p \in [0, \rho(= 2)]$ and for $h \geq 1$, it is the set of frequency vectors of bi-rooted trees T with roots r_1 and r_2, where the frequency vector of the fringe tree rooted at r_2 belongs to $\mathrm{W}^{(0)}_{\mathrm{co}+(\Delta+1)}(\mathtt{a}, d_{\mathtt{a}}, m_{\mathtt{a}}, p; \boldsymbol{x}^*)$ and all other fringe trees are internal fringe trees with the frequency vector of the fringe tree rooted at r_1 belongs to $\mathrm{W}^{(0)}_{(\mathrm{inl})}(\mathtt{a}', d_{\mathtt{a}'} - 1, m''; \boldsymbol{x}^*)$, $m'' < m_{\mathtt{a}'}$ and the length of the path between r_1 and r_2 is $h - \rho$. We give a procedure to compute the set $\mathrm{W}^{(0)}_{\mathrm{co}+(\Delta+1)}(\mathtt{a}, d_{\mathtt{a}}, m_{\mathtt{a}}, \mathtt{a}', d_{\mathtt{a}'}, m_{\mathtt{a}'}, h; \boldsymbol{x}^*)$.

ComputeIntCoreSubtree($\mathtt{a}, d_{\mathtt{a}}, m_{\mathtt{a}}, \mathtt{a}', d_{\mathtt{a}'}, m_{\mathtt{a}'}, h$)

Input: Integer $h \geq 1$, $\Delta \in [2, 3]$, elements $\mathtt{a}, \mathtt{a}' \in \Lambda$,
integers $d_{\mathtt{a}} \in [0, \mathrm{val}(\mathtt{a}) - \Delta - 1]$, $m_{\mathtt{a}} \in [d_{\mathtt{a}}, \mathrm{val}(\mathtt{a}) - \Delta - 1]$, $d_{\mathtt{a}'} \in [1, \mathrm{val}(\mathtt{a}') - 1]$,
$m_{\mathtt{a}'} \in [d_{\mathtt{a}'}, \mathrm{val}(\mathtt{a}') - 1]$.
/* Global data: A vector $\boldsymbol{x}^* = (\boldsymbol{x}^*_{\mathrm{co}}, \boldsymbol{x}^*_{\mathrm{in}}, \boldsymbol{x}^*_{\mathrm{ex}}, b)$ with $\boldsymbol{x}^*_{\mathrm{co}} \in \mathbb{Z}^{\Lambda^{\mathrm{co}}}$, $\boldsymbol{x}^*_{\mathtt{t}} \in \mathbb{Z}^{\Lambda^{\mathtt{t}}}$, $\mathtt{t} \in \{\mathrm{in}, \mathrm{ex}\}$,
a non-negative integer b, the collection $\mathcal{W}^{(0)}_{\mathrm{co}+(\Delta+1)}$ of sets $\mathrm{W}^{(0)}_{\mathrm{co}+(\Delta+1)}(\mathtt{a}, d_{\mathtt{a}}, m_{\mathtt{a}}, p; \boldsymbol{x}^*)$ for $p \leq 2$,
the collection $\mathcal{W}^{(0)}_{\mathrm{inl}}$ of sets $\mathrm{W}^{(0)}_{(\mathrm{inl})}(\mathtt{a}', d_{\mathtt{a}'} - 1, m''; \boldsymbol{x}^*)$, $m'' < m_{\mathtt{a}'}$,
for $h \geq 2$, the collection $\mathcal{W}^{(0,h)}_{\mathrm{co}+(\Delta+1)}$ of vector sets $\mathrm{W}^{(0)}_{\mathrm{co}+(\Delta+1)}(\mathtt{a}, d_{\mathtt{a}}, m_{\mathtt{a}}, \mathtt{b}, d_{\mathtt{b}}, m_{\mathtt{b}}, h-1; \boldsymbol{x}^*)$,
$\mathtt{b} \in \Lambda$, $d_{\mathtt{b}} \in [1, \mathrm{val}(\mathtt{b}) - 1]$, $m_{\mathtt{b}} \in [d_{\mathtt{b}}, \mathrm{val}(\mathtt{b}) - 1]$, integer $g \geq 1$ and
for each vector w in these sets, a set $\mathcal{T}_{\boldsymbol{w}}$ of sample trees $T_{\boldsymbol{w}}$ of size at most g and
and the number $n_{\boldsymbol{w}}$ of samples trees
with vector $\boldsymbol{w}$. */

Output: The set $\mathrm{W}^{(0)}_{\mathrm{co}+(\Delta+1)}(\mathtt{a}, d_{\mathtt{a}}, m_{\mathtt{a}}, \mathtt{a}', d_{\mathtt{a}'}, m_{\mathtt{a}'}, h; \boldsymbol{x}^*)$, where we store each vector
$\boldsymbol{w} \in \mathrm{W}^{(0)}_{\mathrm{co}+(\Delta+1)}(\mathtt{a}, d_{\mathtt{a}}, m_{\mathtt{a}}, \mathtt{a}', d_{\mathtt{a}'}, m_{\mathtt{a}'}, h; \boldsymbol{x}^*)$,
a set $\mathcal{T}_{\boldsymbol{w}}$ of sample trees $T_{\boldsymbol{w}}$ of size at most g and
number $n_{\boldsymbol{w}}$ of trees with vector $\boldsymbol{w}$ in a trie.

W := $\emptyset$;
for each triplet $(\mathtt{a}', d_{\mathtt{a}'} - 1, m'')$ **do**
  if $h = 1$ **then**
    for each $p \in [0, 2]$
      for each $m' \in [1, 3]$
        - $\gamma^{\mathrm{in}} := (\mathtt{a}\{d_{\mathtt{a}} + \Delta\}, \mathtt{a}'\{d_{\mathtt{a}'} + 1\}, m') \in \Gamma^{\mathrm{in}}$ and
        - $m'' + m' = m_{\mathtt{a}'}, m_{\mathtt{a}'} + 1 \leq \mathrm{val}(\mathtt{a}')$, $m_{\mathtt{a}} + m' + \Delta + 1 \leq \mathrm{val}(\mathtt{a})$ **do**
        for each $\boldsymbol{w}_{\mathtt{a}'} \in \mathrm{W}^{(0)}_{(\mathrm{inl})}(\mathtt{a}', d_{\mathtt{a}'} - 1, m''; \boldsymbol{x}^*)$ and
            $\boldsymbol{w}_{\mathtt{a}} \in \mathrm{W}^{(0)}_{\mathrm{co}+(\Delta+1)}(\mathtt{a}, d_{\mathtt{a}}, m_{\mathtt{a}}, p; \boldsymbol{x}^*)$ such that $\boldsymbol{w} := \boldsymbol{w}_{\mathtt{a}} + \boldsymbol{w}_{\mathtt{a}'} + \mathbf{1}_{\gamma^{\mathrm{in}}} \leq \boldsymbol{x}^*$
          if $\boldsymbol{w} \in \mathrm{W}$ **then** $n_{\boldsymbol{w}} = n_{\boldsymbol{w}} + n_{\boldsymbol{w}^{\mathtt{a}}} \cdot n_{\boldsymbol{w}^{\mathtt{a}'}}$
          else
            W := W $\cup \{\boldsymbol{w}\}$; $\mathcal{T}_{\boldsymbol{w}} := \emptyset$; $n_{\boldsymbol{w}} := n_{\boldsymbol{w}^{\mathtt{a}}} \cdot n_{\boldsymbol{w}^{\mathtt{a}'}}$
          end if
          if $\boldsymbol{w} \in \mathrm{W}$ **then**
            for each $T_{\boldsymbol{w}^{\mathtt{a}}} \in \mathcal{T}_{\boldsymbol{w}^{\mathtt{a}}}$ and $T_{\boldsymbol{w}^{\mathtt{a}'}} \in \mathcal{T}_{\boldsymbol{w}^{\mathtt{a}'}}$ **do**

Let T be the tree obtained by joining the roots of $T_{\boldsymbol{w}^{\mathtt{a}}}$ and $T_{\boldsymbol{w}^{\mathtt{a}'}}$
by an edge of multiplicity m';
if $|\mathcal{T}_{\boldsymbol{w}}| < g$ **then** $\mathcal{T}_{\boldsymbol{w}} := \mathcal{T}_{\boldsymbol{w}} \cup \{T\}$
end for
end if
end for
end for
end for
else /* $h \geq 2$ */
for each $(\mathtt{b}, d_{\mathtt{b}}, m_{\mathtt{b}})$
for each $m' \in [1, 3]$
- $\gamma^{\mathrm{in}} := (\mathtt{b}\{d_{\mathtt{b}} + 1\}, \mathtt{a}'\{d_{\mathtt{a}'} + 1\}, m') \in \Gamma^{\mathrm{in}}$ and
- $m'' + m' = m_{\mathtt{a}'}, m_{\mathtt{a}'} + 1 \leq \mathrm{val}(\mathtt{a}')$, $m_{\mathtt{b}} + m' \leq \mathrm{val}(\mathtt{b})$ **do**
for each $\boldsymbol{w}_{\mathtt{a}'} \in \mathrm{W}^{(0)}_{(\mathrm{inl})}(\mathtt{a}', d_{\mathtt{a}'} - 1, m''; \boldsymbol{x}^*)$ and
$\boldsymbol{w}_{\mathtt{a}} \in \mathrm{W}^{(0)}_{\mathrm{co}+(\Delta+1)}(\mathtt{a}, d_{\mathtt{a}}, m_{\mathtt{a}}, p, \mathtt{b}, d_{\mathtt{b}}, m_{\mathtt{b}}, h-1; \boldsymbol{x}^*)$ such that $\boldsymbol{w} := \boldsymbol{w}_{\mathtt{a}} + \boldsymbol{w}_{\mathtt{a}'} + \mathbf{1}_{\gamma^{\mathrm{in}}} \leq \boldsymbol{x}^*$
if $\boldsymbol{w} \in \mathrm{W}$ **then** $n_{\boldsymbol{w}} = n_{\boldsymbol{w}} + n_{\boldsymbol{w}^{\mathtt{a}}} \cdot n_{\boldsymbol{w}^{\mathtt{a}'}}$
else
$\mathrm{W} := \mathrm{W} \cup \{\boldsymbol{w}\}$; $\mathcal{T}_{\boldsymbol{w}} := \emptyset$; $n_{\boldsymbol{w}} := n_{\boldsymbol{w}^{\mathtt{a}}} \cdot n_{\boldsymbol{w}^{\mathtt{a}'}}$
end if
if $\boldsymbol{w} \in \mathrm{W}$ **then**
for each $T_{\boldsymbol{w}^{\mathtt{a}}} \in \mathcal{T}_{\boldsymbol{w}^{\mathtt{a}}}$ and $T_{\boldsymbol{w}^{\mathtt{a}'}} \in \mathcal{T}_{\boldsymbol{w}^{\mathtt{a}'}}$ **do**
Let T be the tree obtained by joining the roots of $T_{\boldsymbol{w}^{\mathtt{a}}}$ and $T_{\boldsymbol{w}^{\mathtt{a}'}}$
by an edge of multiplicity m';
if $|\mathcal{T}_{\boldsymbol{w}}| < g$ **then** $\mathcal{T}_{\boldsymbol{w}} := \mathcal{T}_{\boldsymbol{w}} \cup \{T\}$
end for
end if
end for
end for
end for
end if
end for;
Output W as $\mathrm{W}^{(0)}_{\mathrm{co}+(\Delta+1)}(\mathtt{a}, d_{\mathtt{a}}, m_{\mathtt{a}}, p, \mathtt{a}', d_{\mathtt{a}'}, m_{\mathtt{a}'}, h; \boldsymbol{x}^*)$, and for each $\boldsymbol{w} \in \mathrm{W}$, $\mathcal{T}_{\boldsymbol{w}}$ and $n_{\boldsymbol{w}}$.

1.5 Generating Frequency Vectors of Rooted Core-subtrees

For an integer $h \geq 1$, element $\mathtt{a} \in \Lambda$, integers $\Delta \in [2, 3]$, $d \in [1, \mathrm{val}(\mathtt{a}) - \Delta]$, and $m \in [d, \mathrm{val}(\mathtt{a}) - 1]$ we give a procedure to compute the set $\mathrm{W}^{(0)}_{\mathrm{co}+\Delta}(\mathtt{a}, d, m, h; \boldsymbol{x}^*)$. We use this procedure to compute core-subtrees for e-components only.

ComputCoreSubtreeOne$(\mathtt{a}, d, m, h)$

Input: Element $\mathtt{a} \in \Lambda$, integer $d \in [1, \mathrm{val}(a) - \Delta]$, $m \in [d, \mathrm{val}(a) - 1]$, $h \geq 1$.
/* Global data: A vector $\boldsymbol{x}^* = (\boldsymbol{x}^*_{\mathrm{co}}, \boldsymbol{x}^*_{\mathrm{in}}, \boldsymbol{x}^*_{\mathrm{ex}}, b)$ with $\boldsymbol{x}^*_{\mathrm{co}} \in \mathbb{Z}^{\Lambda^{\mathrm{co}}}$, $\boldsymbol{x}^*_{\mathtt{t}} \in \mathbb{Z}^{\Lambda^{\mathtt{t}}}$, $\mathtt{t} \in \{\mathrm{in}, \mathrm{ex}\}$,

a non-negative integer b, the collection
$\mathcal{W}^{(0)}_{\mathrm{co}+\Delta+1}$ vector sets $\mathrm{W}^{(0)}_{\mathrm{co}+\Delta+1}(\mathtt{a}, d-1, m_{\mathtt{a}}, p; \boldsymbol{x}^*)$, $m_{\mathtt{a}} \in [d-1, \mathrm{val}(\mathtt{a}) - \Delta - 1]$, $p \in [0, 2(=\rho)]$
$\mathcal{W}^{(h-2-1)}_{\mathrm{end}}$ of vector sets $\mathrm{W}^{(h-2-1)}_{\mathrm{end}}(\mathtt{a}_1, d_1, m_1; \boldsymbol{x}^*)$, $\mathtt{a}_1 \in \Lambda$, $d_1 \in [1, \mathrm{val}(\mathtt{a}_1) - 1]$,
$m_1 \in [d_1, \mathrm{val}(\mathtt{a}_1) - 1]$, integer $g \geq 1$ and
for each vector w in these sets, a set $\mathcal{T}_{\boldsymbol{w}}$ of sample trees $T_{\boldsymbol{w}}$ of size at most g and
for each vector w in these sets, and the number $n_{\boldsymbol{w}}$ of samples trees
with vector $\boldsymbol{w}$. */

Output: The set $\mathrm{W}^{(0)}_{\mathrm{co}+\Delta}(\mathtt{a}, d, m, h; \boldsymbol{x}^*)$, where we store each vector $\boldsymbol{w} \in \mathrm{W}^{(0)}_{\mathrm{co}+\Delta}(\mathtt{a}, d, m, h; \boldsymbol{x}^*)$,
for each vector w in these sets, a set $\mathcal{T}_{\boldsymbol{w}}$ of sample trees $T_{\boldsymbol{w}}$ of size at most g and
and number $n_{\boldsymbol{w}}$ of trees with vector $\boldsymbol{w}$ in a trie.

$\mathrm{W} := \emptyset$;
for each triplet $(\mathtt{b}, d_{\mathtt{b}}, m_{\mathtt{b}})$ **do**
  for each triplet $(\mathtt{a}, d-1, m_{\mathtt{a}}, p)$ **do**
    for each $\boldsymbol{w}^{\mathtt{b}} = (\boldsymbol{w}^{\mathtt{b}}_{\mathrm{co}}, \boldsymbol{w}^{\mathtt{b}}_{\mathrm{in}}, \boldsymbol{w}^{\mathtt{b}}_{\mathrm{ex}}, 0) \in \mathrm{W}^{(h-2-1)}_{\mathrm{end}}(\mathtt{b}, d_{\mathtt{b}}, m_{\mathtt{b}}; \boldsymbol{x}^*)$ **do**
      for each $m' \in [1, 3]$ such that
        - $\gamma^{\mathrm{in}} = (\mathtt{a}\{d+\Delta\}, \mathtt{b}\{d_{\mathtt{b}}+1\}, m') \in \Gamma^{\mathrm{in}}$ and
        - $m_{\mathtt{a}} + m' = m, m_{\mathtt{a}} + m' + \Delta \leq \mathrm{val}(\mathtt{a})$ and $m' + m_{\mathtt{b}} \leq \mathrm{val}(\mathtt{b})$ **do**
        for each $\boldsymbol{w}^{\mathtt{a}} = (\boldsymbol{w}^{\mathtt{a}}_{\mathrm{co}}, \boldsymbol{w}^{\mathtt{a}}_{\mathrm{in}}, \boldsymbol{w}^{\mathtt{a}}_{\mathrm{ex}}, 0) \in \mathrm{W}^{(0)}_{\mathrm{inl}}(\mathtt{a}, d-1, m_{\mathtt{a}}, p; \boldsymbol{x}^*)$ **do**
          $\boldsymbol{w}_{\mathrm{in}} := \boldsymbol{w}^{\mathtt{a}}_{\mathrm{in}} + \boldsymbol{w}^{\mathtt{b}}_{\mathrm{in}} + \mathbf{1}_{\gamma^{\mathrm{in}}}$;
          $\boldsymbol{w}_{\mathrm{ex}} := \boldsymbol{w}^{\mathtt{a}}_{\mathrm{ex}} + \boldsymbol{w}^{\mathtt{b}}_{\mathrm{ex}}$; $\boldsymbol{w} := (\boldsymbol{w}_{\mathrm{co}}, \boldsymbol{w}_{\mathrm{in}}, \boldsymbol{w}_{\mathrm{ex}}, 1)$;
          if $\boldsymbol{w} \leq \boldsymbol{x}^*$ **then**
            if $\boldsymbol{w} \in \mathrm{W}$ **then** $n_{\boldsymbol{w}} = n_{\boldsymbol{w}} + n_{\boldsymbol{w}^{\mathtt{a}}} \cdot n_{\boldsymbol{w}^{\mathtt{b}}}$
            else
              $\mathrm{W} := \mathrm{W} \cup \{\boldsymbol{w}\}$; $\mathcal{T}_{\boldsymbol{w}} := \emptyset$; $n_{\boldsymbol{w}} := n_{\boldsymbol{w}^{\mathtt{a}}} \cdot n_{\boldsymbol{w}^{\mathtt{b}}}$
            end if
            if $\boldsymbol{w} \in \mathrm{W}$ **then**
              for each $T_{\boldsymbol{w}^{\mathtt{a}}} \in \mathcal{T}_{\boldsymbol{w}^{\mathtt{a}}}$ and $T_{\boldsymbol{w}^{\mathtt{b}}} \in \mathcal{T}_{\boldsymbol{w}^{\mathtt{b}}}$ **do**
                Let T be the tree obtained by joining the roots of $T_{\boldsymbol{w}^{\mathtt{a}}}$ and $T_{\boldsymbol{w}^{\mathtt{b}}}$
                  by an edge of multiplicity m';
                if $|\mathcal{T}_{\boldsymbol{w}}| < g$ **then** $\mathcal{T}_{\boldsymbol{w}} := \mathcal{T}_{\boldsymbol{w}} \cup \{T\}$
              end for
            end if
          end if
        end for
      end for
    end for
  end for
end for;
Output W as $\mathrm{W}^{(0)}_{\mathrm{co}+\Delta}(\mathtt{a}, d, m, h; \boldsymbol{x}^*)$, and for each $\boldsymbol{w} \in \mathrm{W}$, $\mathcal{T}_{\boldsymbol{w}}$ and $n_{\boldsymbol{w}}$.

1.6 Generation of Frequency Vectors of Bi-rooted Core-subtrees

For an integer $h \in [h_1, h_2]$, elements $\mathtt{a}, \mathtt{a}^e \in \Lambda$, integers $d \in [1, \mathrm{val}(\mathtt{a}) - 1]$, $m \in [d, \mathrm{val}(\mathtt{a}) - 1]$, $\Delta^e \in [1, \mathrm{val}(\mathtt{a}^e) - 1]$, $m^e \leq \mathrm{val}(\mathtt{a}^e) - \Delta^e$, and $q \geq 1$, we give a procedure to compute the set $\mathrm{W}^{(q)}_{\mathrm{co}+1,\Delta^e}(\mathtt{a}, d, m, \mathtt{a}^e, 1, m^e, h; \boldsymbol{x}^*)$.

ComputeBiRootedCoreSubtree$(\mathtt{a}, d, m, \mathtt{a}^e, 1, m^e, h, q)$

Input: An integer $h \geq 0$, elements $\mathtt{a}, \mathtt{a}^e \in \Lambda$, integers $d \in [1, \mathrm{val}(\mathtt{a}) - 1]$, $m \in [d, \mathrm{val}(\mathtt{a}) - 1]$, $\Delta^e \in [1, \mathrm{val}(\mathtt{a}^e) - 1]$, $m^e \leq \mathrm{val}(\mathtt{a}^e) - \Delta^e$, and $q \geq 1$.
/* Global data: A vector $\boldsymbol{x}^* = (\boldsymbol{x}^*_{\mathrm{co}}, \boldsymbol{x}^*_{\mathrm{in}}, \boldsymbol{x}^*_{\mathrm{ex}}, b)$ with $\boldsymbol{x}^*_{\mathrm{co}} \in \mathbb{Z}^{\Lambda^{\mathrm{co}}}$, $\boldsymbol{x}^*_{\mathtt{t}} \in \mathbb{Z}^{\Lambda^{\mathtt{t}}}$, $\mathtt{t} \in \{\mathrm{in}, \mathrm{ex}\}$,
a non-negative integer b, the collection
$\mathcal{W}^{(0)}_{\mathrm{co}+2}$ vector sets $\mathrm{W}^{(0)}_{\mathrm{co}+2}(\mathtt{a}, d-1, m_{\mathtt{a}}, p; \boldsymbol{x}^*)$, $m_{\mathtt{a}} \in [d-1, \mathrm{val}(\mathtt{a}) - \Delta - 1]$, $p \in [0, h]$,
for $q \geq 2$, $\mathcal{W}^{(q-1)}_{\mathrm{end}}$ of vector sets $\mathrm{W}^{(q-1)}_{\mathrm{co}+1,\Delta^e}(\mathtt{b}, d', m', \mathtt{a}^e, 1, m^e, h'; \boldsymbol{x}^*)$,
$\mathtt{b} \in \Lambda$, $d' \in [1, \mathrm{val}(\mathtt{b}) - 1]$, $m' \in [d', \mathrm{val}(\mathtt{b}) - 1]$, $h' \in [0, h]$, integer $g \geq 1$ and
for each vector w in these sets, a set $\mathcal{T}_{\boldsymbol{w}}$ of sample trees $T_{\boldsymbol{w}}$ of size at most g and
and the number $n_{\boldsymbol{w}}$ of samples trees
with vector $\boldsymbol{w}$. */
Output: The set $\mathrm{W}^{(q)}_{\mathrm{co}+1,\Delta^e}(\mathtt{a}, d, m, \mathtt{a}^e, 1, m^e, h; \boldsymbol{x}^*)$, where we store each vector
$\boldsymbol{w} \in \mathrm{W}^{(q)}_{\mathrm{co}+1,\Delta^e}(\mathtt{a}, d, m, \mathtt{a}^e, 1, m^e, h; \boldsymbol{x}^*)$,
a set $\mathcal{T}_{\boldsymbol{w}}$ of sample trees $T_{\boldsymbol{w}}$ of size at most g and
number $n_{\boldsymbol{w}}$ of trees with vector $\boldsymbol{w}$ in a trie.

```
W := ∅;
for each triplet (a, d − 1, m_a, p) do
  if q = 1 then
    if p = h and val(a) ≥ m_a + m^e then
      for each w^a ∈ W^(0)_inl(a, d − 1, m_a, p; x*) do
        γ^co := (ad, a^e 1, m^e); w := w^a + 1_{γ^co}
        if γ^co ∈ Γ^co and w ≤ x* then
          if w ∈ W then n_w = n_w + n_{w^a} · n_{w^b}
          else
            W := W ∪ {w}; T_w := ∅; n_w := n_{w^a} · n_{w^b}
          end if
          if w ∈ W then
            for each T_{w^a} ∈ T_{w^a} and T_{w^b} ∈ T_{w^b} do
              Let T be the tree obtained by joining the roots of T_{w^a} and T_{w^b}
                by an edge of multiplicity m′;
              if |T_w| < g then T_w := T_w ∪ {T}
            end for
          end if
        end if
      end for
    end if
  else /* q > 1 */
```

for each triplet $(\mathtt{b}, d_{\mathtt{b}}, m_{\mathtt{b}}, h')$ **do**
  for each $\boldsymbol{w}^{\mathtt{b}} \in \mathrm{W}^{(q-1)}_{\mathrm{co}+1,\Delta^e}(\mathtt{b}, d_{\mathtt{b}}, m_{\mathtt{b}}, \mathtt{a}^e, 1, m^e, h'; \boldsymbol{x}^*)$ **do**
    for each $m' \in [1, 3]$ such that
      - $\gamma^{\mathrm{co}} := (\mathtt{a}d, \mathtt{b}\{d_{\mathtt{b}} + 1\}, m') \in \Gamma^{\mathrm{co}}$ and
      - $m_{\mathtt{a}} + m' = m, m_{\mathtt{a}} + m' + 1 \leq \mathrm{val}(\mathtt{a}),\ m' + m_{\mathtt{b}} \leq \mathrm{val}(\mathtt{b})$,
      - $h = \max\{p, h'\}$ and
      - $\boldsymbol{w} := \boldsymbol{w}_{\mathtt{a}} + \boldsymbol{w}_{\mathtt{b}} + \mathbf{1}_{\gamma^{\mathrm{co}}} \leq \boldsymbol{x}^*$ **do**
        if $\boldsymbol{w} \in \mathrm{W}$ **then** $n_{\boldsymbol{w}} = n_{\boldsymbol{w}} + n_{\boldsymbol{w}^{\mathtt{a}}} \cdot n_{\boldsymbol{w}^{\mathtt{b}}}$
        else
          $\mathrm{W} := \mathrm{W} \cup \{\boldsymbol{w}\}$; $\mathcal{T}_{\boldsymbol{w}} := \emptyset$; $n_{\boldsymbol{w}} := n_{\boldsymbol{w}^{\mathtt{a}}} \cdot n_{\boldsymbol{w}^{\mathtt{b}}}$
        end if
        if $\boldsymbol{w} \in \mathrm{W}$ **then**
          for each $T_{\boldsymbol{w}^{\mathtt{a}}} \in \mathcal{T}_{\boldsymbol{w}^{\mathtt{a}}}$ and $T_{\boldsymbol{w}^{\mathtt{b}}} \in \mathcal{T}_{\boldsymbol{w}^{\mathtt{b}}}$ **do**
            Let T be the tree obtained by joining the roots of $T_{\boldsymbol{w}^{\mathtt{a}}}$ and $T_{\boldsymbol{w}^{\mathtt{b}}}$
              by an edge of multiplicity m';
            if $|\mathcal{T}_{\boldsymbol{w}}| < g$ **then** $\mathcal{T}_{\boldsymbol{w}} := \mathcal{T}_{\boldsymbol{w}} \cup \{T\}$
          end for
        end if
      end for
    end for
  end for
end if
end for;
Output W as $\mathrm{W}^{(q)}_{\mathrm{co}+1,\Delta^e}(\mathtt{a}, d, m, \mathtt{a}^e, 1, m^e, h; \boldsymbol{x}^*)$, and for each $\boldsymbol{w} \in \mathrm{W}$, $\mathcal{T}_{\boldsymbol{w}}$ and $n_{\boldsymbol{w}}$.

1.7 Computing Feasible Vector Pairs for a v-component

For given $\Delta, \mathtt{a}, d, m, h$ and frequency vector $\boldsymbol{x}^*$ of a v-component, a feasible pair $(\boldsymbol{z}_1, \boldsymbol{z}_2)$ is defined to be vectors $\boldsymbol{z}_1 \in \mathrm{W}^{(0)}_{\mathrm{co}+(\Delta+1)}(\mathtt{a}, d-1, m_{\mathtt{a}}, \mathtt{a}', d_{\mathtt{a}'}, m_{\mathtt{a}'}, \delta_2; \boldsymbol{x}^*)$ and $\boldsymbol{z}_2 \in \mathrm{W}^{(\delta_1)}_{\mathrm{end}}(\mathtt{b}, d', m'; \boldsymbol{x}^*)$, where $\delta_1 = \lfloor \frac{h-2-1}{2} \rfloor$ and $\delta_2 = \lceil \frac{h-2-1}{2} \rceil$, $m_{\mathtt{a}} < m$ such that there exists at least one $\gamma = (\mathtt{b}\{d' + 1\}, \mathtt{a}'\{d_{\mathtt{a}'} + 1\}, m'') \in \Gamma^{\mathrm{in}}$ with $m'' \in [1, \min\{3, \mathrm{val}(\mathtt{a}') - m_{\mathtt{a}'}, \mathrm{val}(\mathtt{b}) - m'\}]$ for which it holds that $\boldsymbol{x}^* = \boldsymbol{z}_1 + \boldsymbol{z}_2 + \mathbf{1}_{\gamma}$. We give a procedure to compute feasible vector pairs for a v-component to generate frequency vectors of rooted core-subtrees $\mathrm{W}^{(0)}_{\mathrm{co}+\Delta}(\mathtt{a}, d, m, h; \boldsymbol{x}^*)$.

Algorithm COMBINEVERTEXCOMP(global data: $\mathtt{a}, d, m, h, \boldsymbol{x}^*$)
Input: A tuple $(\mathtt{a}, d, m, h, \boldsymbol{x}^*)$, two sets W_1 and W_2 such that for $i = 1, 2$,
  $\mathrm{W}_1 = \mathrm{W}^{(0)}_{\mathrm{co}+(\Delta+1)}(\mathtt{a}, d-1, m_{\mathtt{a}}, \mathtt{a}', d_{\mathtt{a}'}, m_{\mathtt{a}'}, \delta_2; \boldsymbol{x}^*)$ and $\mathrm{W}_2 = \mathrm{W}^{(\delta_1)}_{\mathrm{end}}(\mathtt{b}, d', m'; \boldsymbol{x}^*)$,
  where $\delta_1 = \lfloor \frac{h-2-1}{2} \rfloor$ and $\delta_2 = \lceil \frac{h-2-1}{2} \rceil$, $m_{\mathtt{a}} < m$.
Output: All feasible pairs $(\boldsymbol{z}_1, \boldsymbol{z}_2)$ of vectors with $\boldsymbol{z}_i \in \mathrm{W}_i, i = 1, 2$
  and a lower number q on the total number of graph that satisfy all
  feasible pairs of vectors.
$q := 0$;
for each pair of $\gamma = (\mathtt{b}\{d' + 1\}, \mathtt{a}'\{d_{\mathtt{a}'} + 1\}, m'') \in \Gamma^{\mathrm{in}}$ with

$m'' \in [1, \min\{3, \mathrm{val}(\mathtt{a}') - m_{\mathtt{a}'}, \mathrm{val}(\mathtt{b}) - m'\}]$ **do**
Let L_1 denote the sorted list of vectors in W_1;
Construct the set $\overline{\mathrm{W}} := \{\overline{\boldsymbol{z}} \mid \boldsymbol{z} \in \mathrm{W}_2\}$ of the γ-complement vectors;
Sort the vectors in $\overline{\mathrm{W}}$ to obtain a sorted list L_2;
Merge L_1 and L_2 into a single sorted list L_γ of vectors in both lists (as a multiset);
Trace the list L_γ and for each consecutive pair $\boldsymbol{z}^1, \boldsymbol{z}^2$ of vectors with $\boldsymbol{z}^1 = \boldsymbol{z}^2$
Output $(\boldsymbol{z}^1, \overline{\boldsymbol{z}^2})$ as a feasible pair;
Let T be a tree obtained by joining the roots of $T_{\boldsymbol{z}^1}$ and $T_{\overline{\boldsymbol{z}^2}}$ with edge- configuration γ;
$q := q + n_{\boldsymbol{z}^1} \cdot n_{\overline{\boldsymbol{z}^2}}$
endfor;
Output all feasible pairs and q as a lower bound q .

1.8 Computing Feasible Vector Pairs for an e-component

We give a procedure to compute feasible vector pairs.

Algorithm COMBINEEDGECOMP(global data: $\boldsymbol{x}^*, \ell$)
Input: An integer $\ell \geq 2$, two sets W_1 and W_2 such that for $i = 1, 2$,
$\mathrm{W}_i(\mathtt{a}_i, d_i, m_i, \mathtt{a}_i^e, 1, m_i^e, h_i; \boldsymbol{x}^*) = \mathrm{W}^{(\delta_i)}_{\mathrm{co}+1,\Delta_i}(\mathtt{a}_i, d_i, m_i, \mathtt{a}_i^e, 1, m_i^e, h_i; \boldsymbol{x}^*)$,
where $\delta_1 = \lfloor \frac{\ell-1}{2} \rfloor$ and $\delta_2 = \lceil \frac{\ell-1}{2} \rceil$.
Output: All feasible pairs $(\boldsymbol{z}_1, \boldsymbol{z}_2)$ of vectors with $\boldsymbol{z}_i \in \mathrm{W}_i(\mathtt{a}_i, d_i, m_i), i = 1, 2$
and a lower number q on the total number of graph that satisfy all
feasible pairs of vectors.
$q := 0$;
for each pair of $\gamma = (\mathtt{a}_1\{d_1 + 1\}, \mathtt{a}_2\{d_2 + 1\}, m) \in \Gamma^{\mathrm{co}}$ with
$m \in [1, \min\{3, \mathrm{val}(\mathtt{a}_1) - m_1, \mathrm{val}(\mathtt{a}_2) - m_2\}]$ **do**
Let L_1 denote the sorted list of vectors in $\mathrm{W}_1(\mathtt{a}_1, d_1, m_1)$;
Construct the set $\overline{\mathrm{W}} := \{\overline{\boldsymbol{z}} \mid \boldsymbol{z} \in \mathrm{W}_2(\mathtt{a}_2, d_2, m_2)\}$ of the γ-complement vectors;
Sort the vectors in $\overline{\mathrm{W}}$ to obtain a sorted list L_2;
Merge L_1 and L_2 into a single sorted list L_γ of vectors in both lists (as a multiset);
Trace the list L_γ and for each consecutive pair $\boldsymbol{z}^1, \boldsymbol{z}^2$ of vectors with $\boldsymbol{z}^1 = \boldsymbol{z}^2$
Output $(\boldsymbol{z}^1, \overline{\boldsymbol{z}^2})$ as a feasible pair;
Let T be a tree obtained by joining the roots of $T_{\boldsymbol{z}^1}$ and $T_{\overline{\boldsymbol{z}^2}}$ with edge- configuration γ;
$q := q + \lceil (n_{\boldsymbol{z}^1} \cdot n_{\overline{\boldsymbol{z}^2}})/2 \rceil$
endfor;
Output all feasible pairs and q as a lower bound q .

1.9 A Complete Algorithm to compute frequency vectors of v-components

We briefly summarize how to use the procedures described thus far to obtain an algorithm. Our global constants are a frequency vector $\boldsymbol{x}^*_{\mathrm{v}}$ of a v-component rooted at a base vertex v, a fixed tuple $(\mathtt{a}, d, m)$, a lower bound $\mathrm{ch}_{\mathrm{LB}}(v)$ and an upper bound $\mathrm{ch}_{\mathrm{UB}}(v)$ on core height, where we take $\rho = 2$.

CompleteAlgorithmVertex(Global constants: $\mathtt{a}_v, d_v, m_v, \boldsymbol{x}_v^*$, core height bounds)

Let $h := |\Gamma^{\rm in}| + 2$;
Let $\delta_1 := \lfloor (h-2-1)/2 \rfloor$, $\delta_2 := \lceil (h-2-1)/2 \rceil$;
Compute $\mathrm{W}^{(0)}_{\mathrm{co}+\Delta_v}(\mathtt{a}_v, d_v, m_v, h; \boldsymbol{x}_v^*)$ for a fixed $(\mathtt{a}_v, d_v, m_v, \Delta_v)$,
  and for each $h \in [\mathrm{ch}_{\rm LB}(v), \min\{2, \mathrm{ch}_{\rm UB}(v)\}]$ if $\mathrm{ch}_{\rm LB}(v) \le 2$ and $\boldsymbol{x}_v^*(\mathtt{bc}) = 0$;
Compute $\mathrm{W}^{(0)}_{\mathrm{co}+\Delta_v+1}(\mathtt{a}_v, d_v, m, h; \boldsymbol{x}_v^*)$ for a fixed $(\mathtt{a}_v, d_v, \Delta_v)$,
  for each $m \in [d_v - 1, \mathrm{val}(\mathtt{a}_v) - \Delta_v - 1]$, $h \le 2$ if $\mathrm{ch}_{\rm UB}(v) > 2$ and $\boldsymbol{x}_v^*(\mathtt{bc}) = 1$;
Compute $\mathrm{W}^{(0)}_{\rm end}(\mathtt{a}, d, m; \boldsymbol{x}_v^*)$ for each $\mathtt{a} \in \Lambda$, $d \in [1, \mathrm{val}(\mathtt{a}) - 1]$,
  $m \in [d, \mathrm{val}(\mathtt{a}) - 1]$ if $\mathrm{ch}_{\rm UB}(v) > 2$ and $\boldsymbol{x}_v^*(\mathtt{bc}) = 1$;
Compute $\mathrm{W}^{(0)}_{\rm inl}(\mathtt{a}, d, m; \boldsymbol{x}_v^*)$ for each $\mathtt{a} \in \Lambda$, $d \in [0, \mathrm{val}(\mathtt{a}) - 2]$,
  $m \in [d, \mathrm{val}(\mathtt{a}) - 2]$ if $\mathrm{ch}_{\rm UB}(v) > 2$ and $\boldsymbol{x}_v^*(\mathtt{bc}) = 1$;
Compute $\mathrm{W}^{(\delta_1)}_{\rm end}(\mathtt{b}, d', m'; \boldsymbol{x}_v^*)$ for each $\mathtt{b} \in \Lambda$, $d' \in [1, \mathrm{val}(\mathtt{b}) - 1]$,
  $m' \in [d', \mathrm{val}(\mathtt{b}) - 1]$, if $\mathrm{ch}_{\rm UB}(v) > 2$ and $\boldsymbol{x}_v^*(\mathtt{bc}) = 1$;
Compute $\mathrm{W}^{(0)}_{\mathrm{co}+(\Delta+1)}(\mathtt{a}_v, d_v - 1, m_{\mathtt{a}}, \mathtt{a}', d_{\mathtt{a}'}, m_{\mathtt{a}'}, \delta_2; \boldsymbol{x}_v^*)$, for $\Delta \in [2, 3]$, $\mathtt{a}, \mathtt{a}' \in \Lambda$,
  integers $d_{\mathtt{a}} \in [0, \mathrm{val}(\mathtt{a}) - \Delta - 1]$, $m_{\mathtt{a}} \in [d_{\mathtt{a}}, \mathrm{val}(\mathtt{a}) - \Delta - 1]$, $m_{\mathtt{a}_v} < m_v$, $d_{\mathtt{a}'} \in [1, \mathrm{val}(\mathtt{a}') - 1]$,
  $m_{\mathtt{a}'} \in [d_{\mathtt{a}'}, \mathrm{val}(\mathtt{a}') - 1]$, if $\mathrm{ch}_{\rm UB}(v) > 2$ and $\boldsymbol{x}_v^*(\mathtt{bc}) = 1$;
for each two tuples $(\mathtt{a}_v, d_v - 1, m_{\mathtt{a}}, \mathtt{a}', d_{\mathtt{a}'}, m_{\mathtt{a}'}, \delta_2; \boldsymbol{x}_v^*)$, $(\mathtt{b}, d', m'; \boldsymbol{x}_v^*)$ **do**
    search for a feasible vector pair in the pair of sets
    $\mathrm{W}^{(0)}_{\mathrm{co}+(\Delta+1)}(\mathtt{a}_v, d_v - 1, m_{\mathtt{a}}, \mathtt{a}', d_{\mathtt{a}'}, m_{\mathtt{a}'}, \delta_2; \boldsymbol{x}_v^*)$ and $\mathrm{W}^{(\delta_1)}_{\rm end}(\mathtt{b}, d', m'; \boldsymbol{x}_v^*)$
end for.

1.10 A Complete Algorithm to compute frequency vectors of e-components

We briefly summarize how to use the procedures described thus far to obtain an algorithm. Our global constants are a frequency vector $\boldsymbol{x}^*_{\mathrm{e}}$ of an e-component, two fixed tuples $(\mathtt{a}^e_j, m^e_j, \Delta^e_j), j = 1, 2$ a lower bound $\mathrm{ch}_{\mathrm{LB}}(e)$ and an upper bound $\mathrm{ch}_{\mathrm{UB}}(e)$ on core height, where we take $\rho = 2$.

CompleteAlgorithmEdge(Global constants: $\mathtt{a}^e_j, m^e_j, \Delta^e_j, \boldsymbol{x}^*_e$, core height bounds)

$\Gamma^{\mathrm{in}}_e :=$ The set internal edges in $\boldsymbol{x}^*_e$;
Compute $\mathrm{W}^{(0)}_{\mathrm{co}+\Delta}(\mathtt{a}, d, m, h; \boldsymbol{x}^*_e)$ for each
  $\Delta \in [2, 3]$, $\mathtt{a} \in \Lambda$, $d \in [0, \mathrm{val}(\mathtt{a}) - \Delta]$, $m \in [d, \mathrm{val}(\mathtt{a}) - \Delta]$, $h \in [0, \min\{2, \mathrm{ch}_{\mathrm{UB}}(e)\}]$;
Compute $\mathrm{W}^{(0)}_{\mathrm{end}}(\mathtt{a}, d, m; \boldsymbol{x}^*_e)$ for each $\mathtt{a} \in \Lambda$, $d \in [1, \mathrm{val}(\mathtt{a}) - 1]$, $m \in [d, \mathrm{val}(\mathtt{a}) - 1]$;
Compute $\mathrm{W}^{(0)}_{\mathrm{inl}}(\mathtt{a}, d, m; \boldsymbol{x}^*_e)$ for each $\mathtt{a} \in \Lambda$, $d \in [0, \mathrm{val}(\mathtt{a}) - 2]$, $m \in [d, \mathrm{val}(\mathtt{a}) - 2]$;
Compute $\mathrm{W}^{(h)}_{\mathrm{end}}(\mathtt{a}, d, m; \boldsymbol{x}^*_e)$ for each $\mathtt{a} \in \Lambda$, $d \in [1, \mathrm{val}(\mathtt{a}) - 1]$,
  $m \in [d, \mathrm{val}(\mathtt{a}) - 1]$, $h = \min\{|\Gamma^{\mathrm{in}}_e| - 1, \mathrm{ch}_{\mathrm{UB}}(e) - 2 - 1\}$ if $\mathrm{ch}_{\mathrm{UB}}(e) > 2$;
Compute $\mathrm{W}^{(0)}_{\mathrm{co}+\Delta}(\mathtt{a}, d, m, h; \boldsymbol{x}^*_v)$ for each $\Delta \in [2, 3]$, $\mathtt{a} \in \Lambda$, $d \in [1, \mathrm{val}(\mathtt{a}) - 1]$,
  $m \in [d, \mathrm{val}(\mathtt{a}) - 1]$, $h = \min\{|\Gamma^{\mathrm{in}}_e| + 2, \mathrm{ch}_{\mathrm{UB}}(e)\}$, if $\mathrm{ch}_{\mathrm{UB}}(e) > 2$;
Compute $\mathrm{W}^{(q)}_{\mathrm{co}+1,\Delta^e_j}(\mathtt{a}, d, m, \mathtt{a}^e_j, 1, m^e_j, h; \boldsymbol{x}^*_e)$ for fixed $(\mathtt{a}^e_j, m^e_j, \Delta^e_j)$, $\mathtt{a}, \in \Lambda$,
  integers $d \in [1, \mathrm{val}(\mathtt{a}) - 1]$, $m \in [d, \mathrm{val}(\mathtt{a}) - 1]$, $q = \Delta^e_j, j = 1, 2$;
for each two tuples $(\mathtt{a}_j, d_j, m_j, \mathtt{a}^e_j, 1, m^e_j, h; \boldsymbol{x}^*_e)$, $j = 1, 2$ **do**
  search for a feasible vector pair in the pair of sets $\mathrm{W}^{(q)}_{\mathrm{co}+1,\Delta^e_j}(\mathtt{a}_j, d_j, m_j, \mathtt{a}^e_j, 1, m^e_j, h_j; \boldsymbol{x}^*_e)$
end for.

1.11 A Complete Algorithm to compute frequency vectors of isomers of a given graph $G^\dagger$

We briefly summarize how to use the procedures described thus far to obtain an algorithm. Our global constants are a graph $G^\dagger$, a path partition $\mathcal{P} = \{P_1, P_2, \ldots, P_p\}$, and for each base-vertex t or base-edge t, a lower bound $\mathrm{ch}_{\mathrm{LB}}(t)$ and an upper bound $\mathrm{ch}_{\mathrm{UB}}(t)$ on core height,where we take $\rho = 2$.

CompleteAlgorithm(Global constants: $G^\dagger, \mathcal{P}$, core height bounds)

Let $\ell_i := \ell(P_i)$ for each $i \in [1, p]$;
Let $\delta_1^i := \lfloor(\ell_i - 1)/2\rfloor$, $\delta_2^i := \lceil(\ell_i - 1)/2\rceil$ for each $i \in [1, p]$;
Compute frequency vector $\boldsymbol{x}_t^*$ for each base-vertex t or and base-edge t;
for each base-vertex $v \in V_B$
  Let $h := |\Gamma^{\mathrm{in}}| + 2$;
  Let $\delta_1' := \lfloor(h - 2 - 1)/2\rfloor$, $\delta_2' := \lceil(h - 2 - 1)/2\rceil$;
  Compute $\mathrm{W}^{(0)}_{\mathrm{co}+\Delta_v}(\mathtt{a}_v, d_v, m_v, h; \boldsymbol{x}_v^*)$ for a fixed $(\mathtt{a}_v, d_v, m_v, \Delta_v)$,
   and for each $h \in [\mathrm{ch}_{\mathrm{LB}}(v), \min\{2, \mathrm{ch}_{\mathrm{UB}}(v)\}]$ if $\mathrm{ch}_{\mathrm{LB}}(v) \leq 2$ and $\boldsymbol{x}_v^*(\mathtt{bc}) = 0$;
  Compute $\mathrm{W}^{(0)}_{\mathrm{co}+\Delta_v+1}(\mathtt{a}_v, d_v, m, h; \boldsymbol{x}_v^*)$ for a fixed $(\mathtt{a}_v, d_v, \Delta_v)$,
   for each $m \in [d_v - 1, \mathrm{val}(\mathtt{a}_v) - \Delta_v - 1]$, $h \leq 2$ if $\mathrm{ch}_{\mathrm{UB}}(v) > 2$ and $\boldsymbol{x}_v^*(\mathtt{bc}) = 1$;
  Compute $\mathrm{W}^{(0)}_{\mathrm{end}}(\mathtt{a}, d, m; \boldsymbol{x}_v^*)$ for each $\mathtt{a} \in \Lambda$, $d \in [1, \mathrm{val}(\mathtt{a}) - 1]$,
   $m \in [d, \mathrm{val}(\mathtt{a}) - 1]$ if $\mathrm{ch}_{\mathrm{UB}}(v) > 2$ and $\boldsymbol{x}_v^*(\mathtt{bc}) = 1$;
  Compute $\mathrm{W}^{(\delta_1')}_{\mathrm{end}}(\mathtt{b}, d', m'; \boldsymbol{x}_v^*)$ for each $\mathtt{b} \in \Lambda$, $d' \in [1, \mathrm{val}(\mathtt{b}) - 1]$,
   $m' \in [d', \mathrm{val}(\mathtt{b}) - 1]$, if $\mathrm{ch}_{\mathrm{UB}}(v) > 2$ and $\boldsymbol{x}_v^*(\mathtt{bc}) = 1$;
  Compute $\mathrm{W}^{(0)}_{\mathrm{co}+(\Delta+1)}(\mathtt{a}_v, d_v - 1, m_{\mathtt{a}}, \mathtt{a}', d_{\mathtt{a}'}, m_{\mathtt{a}'}, \delta_2'; \boldsymbol{x}_v^*)$, for $\Delta \in [2, 3]$, $\mathtt{a}, \mathtt{a}' \in \Lambda$,
   integers $d_{\mathtt{a}} \in [0, \mathrm{val}(\mathtt{a}) - \Delta - 1]$, $m_{\mathtt{a}} \in [d_{\mathtt{a}}, \mathrm{val}(\mathtt{a}) - \Delta - 1]$, $m_{\mathtt{a}_v} < m_v$, $d_{\mathtt{a}'} \in [1, \mathrm{val}(\mathtt{a}') - 1]$,
   $m_{\mathtt{a}'} \in [d_{\mathtt{a}'}, \mathrm{val}(\mathtt{a}') - 1]$, if $\mathrm{ch}_{\mathrm{UB}}(v) > 2$ and $\boldsymbol{x}_v^*(\mathtt{bc}) = 1$;
  for each two tuples $(\mathtt{a}_v, d_v - 1, m_{\mathtt{a}}, \mathtt{a}', d_{\mathtt{a}'}, m_{\mathtt{a}'}, \delta_2'; \boldsymbol{x}_v^*)$, $(\mathtt{b}, d', m'; \boldsymbol{x}_v^*)$ **do**
    search for a feasible vector pair in the pair of sets
    $\mathrm{W}^{(0)}_{\mathrm{co}+(\Delta+1)}(\mathtt{a}_v, d_v - 1, m_{\mathtt{a}}, \mathtt{a}', d_{\mathtt{a}'}, m_{\mathtt{a}'}, \delta_2'; \boldsymbol{x}_v^*)$ and $\mathrm{W}^{(\delta_1')}_{\mathrm{end}}(\mathtt{b}, d', m'; \boldsymbol{x}_v^*)$
  end for
end for;
for each base-edge $e \in E_B$
  Compute $\mathrm{W}^{(0)}_{\mathrm{co}+\Delta}(\mathtt{a}, d, m, h; \boldsymbol{x}_e^*)$ for each
    $\Delta \in [2, 3]$, $\mathtt{a} \in \Lambda$, $d \in [0, \mathrm{val}(\mathtt{a}) - \Delta]$, $m \in [d, \mathrm{val}(\mathtt{a}) - \Delta]$, $h \in [0, \min\{2, \mathrm{ch}_{\mathrm{UB}}(e)\}]$;
  Compute $\mathrm{W}^{(0)}_{\mathrm{end}}(\mathtt{a}, d, m; \boldsymbol{x}_e^*)$ for each $\mathtt{a} \in \Lambda$, $d \in [1, \mathrm{val}(\mathtt{a}) - 1]$, $m \in [d, \mathrm{val}(\mathtt{a}) - 1]$;
  Compute $\mathrm{W}^{(0)}_{\mathrm{inl}}(\mathtt{a}, d, m; \boldsymbol{x}_e^*)$ for each $\mathtt{a} \in \Lambda$, $d \in [0, \mathrm{val}(\mathtt{a}) - 2]$, $m \in [d, \mathrm{val}(\mathtt{a}) - 2]$;
  $\Gamma_e^{\mathrm{in}} :=$ number of internal edges in $\boldsymbol{x}_e^*$;
  Compute $\mathrm{W}^{(h)}_{\mathrm{end}}(\mathtt{a}, d, m; \boldsymbol{x}_e^*)$ for each $\mathtt{a} \in \Lambda$, $d \in [1, \mathrm{val}(\mathtt{a}) - 1]$,
   $m \in [d, \mathrm{val}(\mathtt{a}) - 1]$, $h = \min\{|\Gamma_e^{\mathrm{in}}| - 1, \mathrm{ch}_{\mathrm{UB}}(e) - 2 - 1\}$ if $\mathrm{ch}_{\mathrm{UB}}(e) > 2$;
  Compute $\mathrm{W}^{(0)}_{\mathrm{co}+\Delta}(\mathtt{a}, d, m, h; \boldsymbol{x}_v^*)$ for each $\Delta \in [2, 3]$, $\mathtt{a} \in \Lambda$, $d \in [1, \mathrm{val}(\mathtt{a}) - 1]$,
   $m \in [d, \mathrm{val}(\mathtt{a}) - 1]$, $h = \min\{|\Gamma_e^{\mathrm{in}}| + 2, \mathrm{ch}_{\mathrm{UB}}(e)\}$, if $\mathrm{ch}_{\mathrm{UB}}(e) > 2$;
  Compute $\mathrm{W}^{(q)}_{\mathrm{co}+1,\Delta_j^e}(\mathtt{a}, d, m, \mathtt{a}_j^e, 1, m_j^e, h; \boldsymbol{x}_e^*)$ for fixed $(\mathtt{a}_j^e, m_j^e, \Delta_j^e)$, $\mathtt{a}, \in \Lambda$,

integers $d \in [1, \mathrm{val}(\mathtt{a}) - 1]$, $m \in [d, \mathrm{val}(\mathtt{a}) - 1]$, $q = \Delta_j^e, j = 1, 2$;
for each two tuples $(\mathtt{a}_j, d_j, m_j, \mathtt{a}_j^e, 1, m_j^e, h; \boldsymbol{x}_e^*)$, $j = 1, 2$ **do**
search for a feasible vector pair in the pair of sets $\mathrm{W}^{(q)}_{\mathrm{co}+1,\Delta_j^e}(\mathtt{a}_j, d_j, m_j, \mathtt{a}_j^e, 1, m_j^e, h_j; \boldsymbol{x}_e^*)$
/* We store feasible pairs with $\max\{h_1, h_2\} = \mathrm{ch}(G^\dagger)$ and
feasible pairs $\max\{h_1, h_2\} \neq \mathrm{ch}(G^\dagger)$ in different sets */
end for
end for.