Pseudo-codes for Graph Search Algorithm in "A Novel Method for Inference of Acyclic Chemical Compounds with Bounded Branch-height Based on Artificial Neural Networks and Integer Programming"

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 $(\alpha(v_1), \beta(v_{\mathrm{pred}(2)} v_2), \alpha(v_2),$ $\ldots, \beta(v_{\mathrm{pred}(n)} v_n), \alpha(v_n))$ the *sequence representation* of G.

For a given resource vector $\boldsymbol{z} = (\boldsymbol{z}_{\mathrm{in}}, \boldsymbol{z}_{\mathrm{ex}})$ with $\boldsymbol{z}_{\mathrm{in}}, \boldsymbol{z}_{\mathrm{ex}} \in \mathbb{Z}^{\Lambda \cup \Gamma \cup \mathrm{Bc} \cup \mathrm{Dg}}$ and an integer δ, let $\mathcal{W}^{(\delta)}(\boldsymbol{z})$ denote the set of vectors $\boldsymbol{w} = (\boldsymbol{w}_{\mathrm{in}}, \boldsymbol{w}_{\mathrm{ex}})$ with $\boldsymbol{w}_{\mathrm{in}}, \boldsymbol{w}_{\mathrm{ex}} \in \mathbb{Z}^{\Lambda \cup \Gamma \cup \mathrm{Bc} \cup \mathrm{Dg}}$ such that $\boldsymbol{w} \leq \boldsymbol{z}$ and there exists a chemical tree T on $\delta + 1$ vertices such that $\boldsymbol{f}_{\mathrm{in}}(T) = \boldsymbol{w}_{\mathrm{in}}$ and $\boldsymbol{f}_{\mathrm{ex}}(T) = \boldsymbol{w}_{\mathrm{ex}}$ and T is $\boldsymbol{x}^*$-extensible, i.e., T satisfies the condition of Lemma **??**(ii).

Next we give an algorithm that for a given vector $\boldsymbol{x}^* = (\boldsymbol{x}^*_{\mathrm{in}}, \boldsymbol{x}^*_{\mathrm{ex}})$ with $\boldsymbol{x}^*_{\mathrm{in}}, \boldsymbol{x}^*_{\mathrm{ex}} \in \mathbb{Z}^{\Lambda \cup \Gamma \cup \mathrm{Bc} \cup \mathrm{Dg}}$ and an integer δ, calculates the set $\mathcal{W}^{(\delta)}(\boldsymbol{x}^*)$ by constructing sequence representations of chemical graphs.

Algorithm SeqMap($\boldsymbol{x}^*, \delta$)
Input: A vector $\boldsymbol{x}^* = (\boldsymbol{x}^*_{\mathrm{in}}, \boldsymbol{x}^*_{\mathrm{ex}})$ with $\boldsymbol{x}^*_{\mathrm{in}}, \boldsymbol{x}^*_{\mathrm{ex}} \in \mathbb{Z}^{\Lambda \cup \Gamma \cup \mathrm{Bc} \cup \mathrm{Dg}}$, an integer δ.
Output: The set $\mathcal{W}^{(\delta)}(\boldsymbol{x}^*)$ of vectors and a set of sequence representations
  that contains all sequence representation of an acyclic graph G
  with $\boldsymbol{f}_{\mathtt{t}}(G) = \boldsymbol{w}^G_{\mathtt{t}}$, $\mathtt{t} \in \{\mathrm{in}, \mathrm{ex}\}$, for each vector $\boldsymbol{w}^G \in \mathcal{W}^{(\delta)}(\boldsymbol{x}^*)$,
  where the set of these sequences is stored in a trie.
Let $\boldsymbol{nb}[\mathtt{a}] := \sum_{\gamma = (\mathtt{a}, \mathtt{b}, k) \in \Gamma : \mathtt{b} \neq \mathtt{a} \in \Lambda} \boldsymbol{x}^*_{\mathrm{ex}}(\gamma) + 2 \sum_{\gamma = (\mathtt{a}, \mathtt{a}, k) \in \Gamma} \boldsymbol{x}^*_{\mathrm{ex}}(\gamma)$ **for each** element $\mathtt{a} \in \Lambda$ with $\boldsymbol{x}^*_{\mathrm{ex}}(\mathtt{a}) \geq 1$;
for each $t = \mathtt{a} \in \Lambda$ **do**
  $\mathrm{Cld}_t := \mathrm{Leaf}_t := \emptyset$;
  for each tuple $\gamma \in \Gamma$ such that $\gamma = (\mathtt{a}, \mathtt{b}, k)$ for some $\mathtt{b} \in \Lambda$ and $k \in [1, 3]$ **do**
    if $\boldsymbol{x}^*_{\mathrm{ex}}(\mathtt{b}) \geq 1$, $\boldsymbol{x}^*_{\mathrm{ex}}(\gamma) \geq 1$ and $\boldsymbol{x}^*_{\mathrm{in}}(\mathtt{a}) \geq 1$ **then**
      Set $\boldsymbol{w}^0 = (\boldsymbol{w}^0_{\mathrm{in}}, \boldsymbol{w}^0_{\mathrm{ex}})$ with $\boldsymbol{w}^0_{\mathrm{in}}, \boldsymbol{w}^0_{\mathrm{ex}} \in \mathbb{Z}_+^{\Lambda \cup \Gamma \cup \mathrm{Bc} \cup \mathrm{Dg}}$ to be the vector such that all entries are 0;
      if Trie($k, \mathtt{b}, \boldsymbol{w}^0_{\mathrm{in}} + \mathbf{1}_{\mathtt{a}}, \boldsymbol{w}^0_{\mathrm{ex}} + \mathbf{1}_{\mathtt{b}} + \mathbf{1}_{\gamma}, \boldsymbol{nb} - \mathbf{1}_{\mathtt{b}}, \delta - 1$) 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
    endif
  endfor;
  if $\mathrm{Cld}_t \neq \emptyset$ **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 $\mathrm{key}(u) = (\boldsymbol{w}_u, \mathtt{a}_u, h_u)$;
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 $\mathrm{key}(u) = (\boldsymbol{w}_u, \mathtt{a}_u, h_u)$ for a leaf $u \in \mathrm{Leaf}_t^{(i)}$
endif;
Set $\mathrm{W}^{(\delta)}[\boldsymbol{x}^*, t]$ to be the set of vectors $\boldsymbol{w} = \mathrm{key}_1(u_{t,i})$ for all superleaves $u_{t,i}$
endfor;
Output $\{\mathrm{W}^{(\delta)}[\boldsymbol{x}^*, t] \mid t \in \Lambda\}$ as $\mathcal{W}^{(\delta)}(\boldsymbol{x}^*)$.

Recursive Procedure $\textsc{Trie}(h, \mathtt{a}, \boldsymbol{w}, \boldsymbol{nb}, \delta)$
Input: A vector $\boldsymbol{x}^* = (\boldsymbol{x}^*_{\mathrm{in}}, \boldsymbol{x}^*_{\mathrm{ex}})$ with $\boldsymbol{x}^*_{\mathrm{in}}, \boldsymbol{x}^*_{\mathrm{ex}} \in \mathbb{Z}^{\Lambda\cup\Gamma\cup\mathrm{Bc}\cup\mathrm{Dg}}$ (a global constant),
an integer $h \in [1, 3]$, an element $\mathtt{a} \in \Lambda$,
a vector $\boldsymbol{w} = (\boldsymbol{w}_{\mathrm{in}}, \boldsymbol{w}_{\mathrm{ex}})$ with $\boldsymbol{w}_{\mathrm{in}}, \boldsymbol{w}_{\mathrm{ex}} \in \mathbb{Z}_+^{\Lambda\cup\Gamma\cup\mathrm{Bc}\cup\mathrm{Dg}}$,
a vector $\boldsymbol{nb} \in \mathbb{Z}_+^{\Lambda}$, and an integer $\delta \geq 0$.
Output: The set $\{\boldsymbol{w}^G = (\boldsymbol{w}^G_{\mathrm{in}}, \boldsymbol{w}^G_{\mathrm{ex}}) \in \mathcal{W}^{(\delta)}(\boldsymbol{x}^*) \mid \boldsymbol{w}^G_{\mathrm{ex}} \geq \boldsymbol{w}_{\mathrm{ex}}\}$ of vectors and a set of sequence
representations of chemical graphs that contains all graphs G on $\delta + 1$ vertices
rooted at atom $\mathtt{a}$, 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 ($j \in [1, \mathrm{val}(\mathtt{a}) - h]$) under resource bounds of $\boldsymbol{x}^* - \boldsymbol{w}$;
if $\delta = 0$ **then**
Create a new leaf node u with $\mathrm{key}(u) = (\boldsymbol{w}, \mathtt{a}, h)$, return u and a leaf set $\mathrm{Leaf} := \{u\}$
else
$\mathrm{Cld} := \mathrm{Leaf} := \emptyset$;
for each tuple $\gamma = (\mathtt{a}, \mathtt{b}, k) \in \Gamma$ **do**
if $h + k \leq \mathrm{val}(\mathtt{a})$, $\boldsymbol{w}_{\mathrm{ex}}(\mathtt{b}) < \boldsymbol{x}^*_{\mathrm{ex}}(\mathtt{b})$, $\boldsymbol{w}_{\mathrm{ex}}(\gamma) < \boldsymbol{x}^*_{\mathrm{ex}}(\gamma)$,
$\boldsymbol{x}^*_{\mathrm{ex}}(\mathtt{a}) - \boldsymbol{w}_{\mathrm{ex}}(\mathtt{a}) \leq \boldsymbol{nb}[\mathtt{a}] - 1$ **then**
if $\textsc{Trie}(k + h, \mathtt{b}, \boldsymbol{w}_{\mathrm{in}}, \boldsymbol{w}_{\mathrm{ex}} + \mathbf{1}_{\mathtt{b}} + \mathbf{1}_{\gamma} + \mathbf{1}_{\mu}, \boldsymbol{nb} - \mathbf{1}_{\mathtt{a}} - \mathbf{1}_{\mathtt{b}}, \delta - 1)$ 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
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 $\boldsymbol{x}^* = (\boldsymbol{x}^*_{\rm in}, \boldsymbol{x}^*_{\rm ex})$.

FRINGETREEWEIGHTVECTORS($\mathtt{a}$)
Input: A vector $\boldsymbol{x}^* = (\boldsymbol{x}^*_{\rm in}, \boldsymbol{x}^*_{\rm ex})$ with $\boldsymbol{x}^*_{\rm in}, \boldsymbol{x}^*_{\rm ex} \in \mathbb{Z}_+^{\Lambda\cup\Gamma\cup{\rm Bc}\cup{\rm Dg}}$ and
an element $\mathtt{a} \in \Lambda$ such that $\boldsymbol{x}^*_{\rm in}[\mathtt{a}] \geq 1$;
Output: The sets ${\rm W}^{(0)}_{\rm end}(\mathtt{a}, d, m)$ (resp., ${\rm W}^{(0)}_{\rm inl}(\mathtt{a}, d, m)$ and ${\rm W}^{(0)}_{\rm inl+3}(\mathtt{a}, d, m)$)
$d \in [1, {\rm val}(\mathtt{a}) - 1]$ (resp., $d \in [0, {\rm val}(\mathtt{a}) - 2]$ and $d \in [0, {\rm val}(\mathtt{a}) - 3]$) and
$m \in [d, {\rm val}(\mathtt{a}) - 1]$ (resp., $m \in [d, {\rm val}(\mathtt{a}) - 2]$ and $m \in [d, {\rm val}(\mathtt{a}) - 3]$)
and for each vector $\boldsymbol{w}$ in these sets, one sample tree $T_{\boldsymbol{w}}$ and the number $n_{\boldsymbol{w}}$ of all sample trees.
Step 1: Enumerate all fringe-trees T rooted at vertex v_r such that
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),
$\boldsymbol{f}_{\rm ex}(T) \leq \boldsymbol{x}^*_{\rm ex}$ and $\boldsymbol{f}_{\rm in}(T) = \boldsymbol{0} + \boldsymbol{1}_{\mathtt{a}}$,
the degree d_c of child v_c and the multiplicity k of edge $e_{\rm root} = v_r v_c$
satisfy the following:
$\boldsymbol{f}_{\rm ex\,[Bc]}(T) - \boldsymbol{1}_\mu \leq \boldsymbol{x}^*_{\rm ex\,[Bc]}$ for the bond-configuration $\mu = (1, d_c, k)$ of edge $e_{\rm root}$;
/* Using recursive algorithm SEQMAP to enumerate these */
Let $\mathcal{T} = \{(T_i, k_i, d_i, \boldsymbol{w}^i_{\rm in}, \boldsymbol{w}^i_{\rm ex}) \mid i = 1, 2, \ldots, q\}$ 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
$\boldsymbol{w}^i_{\rm ex} = \boldsymbol{f}_{\rm ex}(T_i) - \boldsymbol{1}_\mu$ for the bond-configuration μ of edge $e_{\rm root} = v_r v_c$;

Step 2: Enumerate all fringe-trees T with $d_{\rm root} \in [1, 2, 3]$ as follows:
${\rm W}[\mathtt{a}, d, m] := \emptyset$ for $d \in [1, {\rm val}(\mathtt{a}) - 1]$, $m \in [d, {\rm val}(a) - d]$;
Let ${\rm dg}^+ := 1$ (resp., ${\rm dg}^+ := 2$ and ${\rm dg}^+ := 3$);
/* ${\rm dg}^+ := 3$ is used for the case of three leaf 2-branches */
for each $i \in [1, q]$ **do**
if $|V(T_i)| \leq 4$, $\boldsymbol{w}^i_{\rm in} + \boldsymbol{1}_{{\rm dg}^+ + 1} \leq \boldsymbol{x}^*_{\rm in}$ and $\boldsymbol{w}^i_{\rm ex} + \boldsymbol{1}_{\mu(i)} \leq \boldsymbol{x}^*_{\rm ex}$ hold for $\mu(i) := (d_i, {\rm dg}^+ + 1, k_i)$ **then**
/* Also test if the height of the tree T_i is exactly equal to 2 while
constructing ${\rm W}^{(0)}_{\rm end}(a, d, m)$ */
Let $\boldsymbol{w} := (\boldsymbol{w}^i_{\rm in} + \boldsymbol{1}_{{\rm dg}^+ + 1}, \boldsymbol{w}^i_{\rm ex} + \boldsymbol{1}_{\mu(i)})$;
if $\boldsymbol{w} \in {\rm W}[\mathtt{a}, 1, k_i]$ **then** $n_{\boldsymbol{w}} := n_{\boldsymbol{w}} + 1$
else ${\rm W}[\mathtt{a}, 1, k_i] := {\rm W}[\mathtt{a}, 1, k_i] \cup \{\boldsymbol{w}\}$; $T_{\boldsymbol{w}} := T_i$; $n_{\boldsymbol{w}} := 1$ **endif**
endif;
for each $j \in [i, q]$ **do**
if $k_i + k_j \leq {\rm val}(\mathtt{a}) - {\rm dg}^+$ **then**
for each $h \in [j, q]$ **do**

$\mu(i) := (d_i, \mathrm{dg}^+ + 3, k_i)$; $\mu(j) := (d_j, \mathrm{dg}^+ + 3, k_j)$; $\mu(h) := (d_h, \mathrm{dg}^+ + 3, k_h)$;
if $k_i + k_j + k_h \leq \mathrm{val}(\mathtt{a}) - \mathrm{dg}^+$ (i.e., $k_i = k_j = k_h = 1$ and $\mathrm{val}(\mathtt{a}) = 4$),
$\boldsymbol{w}^i_{\mathrm{in}} + \boldsymbol{w}^j_{\mathrm{in}} + \boldsymbol{w}^h_{\mathrm{in}} + \mathbf{1}_{\mathrm{dg}^++3} - \mathbf{1}_{\mathtt{a}} - \mathbf{1}_{\mathtt{a}} \leq \boldsymbol{x}^*_{\mathrm{in}}$, $\boldsymbol{w}^i_{\mathrm{ex}} + \boldsymbol{w}^j_{\mathrm{ex}} + \boldsymbol{w}^h_{\mathrm{ex}} + \mathbf{1}_{\mu(i)} + \mathbf{1}_{\mu(j)} + \mathbf{1}_{\mu(h)} \leq \boldsymbol{x}^*_{\mathrm{ex}}$
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 $\mathrm{W}^{(0)}_{\mathrm{end}}(a, d, m)$ */
$\boldsymbol{w} := (\boldsymbol{w}^i_{\mathrm{in}} + \boldsymbol{w}^j_{\mathrm{in}} + \boldsymbol{w}^h_{\mathrm{in}} + \mathbf{1}_{\mathrm{dg}^++3} - \mathbf{1}_{\mathtt{a}} - \mathbf{1}_{\mathtt{a}}, \boldsymbol{w}^i_{\mathrm{ex}} + \boldsymbol{w}^j_{\mathrm{ex}} + \boldsymbol{w}^h_{\mathrm{ex}} + \mathbf{1}_{\mu(i)} + \mathbf{1}_{\mu(j)} + \mathbf{1}_{\mu(h)})$;
Let T be the tree obtained by identifying the roots of T_i, T_j, and T_h;
Let $\boldsymbol{nb}[\mathtt{a}] := \sum_{\gamma=(\mathtt{a},\mathtt{b},k)\in\Gamma:\mathtt{b}\neq\mathtt{a}\in\Lambda} (\boldsymbol{x}^*_{\mathrm{ex}}(\gamma) - \boldsymbol{f}(\gamma; T)) + 2 \sum_{\gamma=(\mathtt{a},\mathtt{a},k)\in\Gamma} (\boldsymbol{x}^*_{\mathrm{ex}}(\gamma) - \boldsymbol{f}(\gamma; T))$ **for each** $\mathtt{a} \in \Lambda$;
if $\boldsymbol{x}^*_{\mathrm{ex}}(\mathtt{a}) - \boldsymbol{f}_{\mathrm{ex}}(\mathtt{a}; T) \leq \boldsymbol{nb}[\mathtt{a}]$ **for each** $a \in \Lambda$ **then**
$m := k_i + k_j + k_h$;
if $\boldsymbol{w} \in \mathrm{W}[\mathtt{a}, 3, m]$ **then** $n_{\boldsymbol{w}}$+= 1
else
$\mathrm{W}[\mathtt{a}, 3, m] := \mathrm{W}[\mathtt{a}, 3, m] \cup \{\boldsymbol{w}\}$; $T_{\boldsymbol{w}} := T$; $n_{\boldsymbol{w}} := 1$;
endif
endif
endif
endfor;
$\mu(i) := (d_i, \mathrm{dg}^+ + 2, k_i)$; $\mu(j) := (d_j, \mathrm{dg}^+ + 2, k_j)$;
if $|V(T_i)| + |V(T_j)| - 1 \leq 6$, $\boldsymbol{w}^i_{\mathrm{in}} + \boldsymbol{w}^j_{\mathrm{in}} + \mathbf{1}_{\mathrm{dg}^++2} - \mathbf{1}_{\mathtt{a}} \leq \boldsymbol{x}^*_{\mathrm{in}}$,
$\boldsymbol{w}^i_{\mathrm{ex}} + \boldsymbol{w}^j_{\mathrm{ex}} + \mathbf{1}_{\mu(i)} + \mathbf{1}_{\mu(j)} \leq \boldsymbol{x}^*_{\mathrm{ex}}$ **then**
/* Also test if the height of at least one tree T_i, T_j is exactly equal to 2 while
constructing $\mathrm{W}^{(0)}_{\mathrm{end}}(a, d, m)$ */
$\boldsymbol{w} := (\boldsymbol{w}^i_{\mathrm{in}} + \boldsymbol{w}^j_{\mathrm{in}} + \mathbf{1}_{\mathrm{dg}^++2} - \mathbf{1}_{\mathtt{a}}, \boldsymbol{w}^i_{\mathrm{ex}} + \boldsymbol{w}^j_{\mathrm{ex}} + \mathbf{1}_{\mu(i)} + \mathbf{1}_{\mu(j)})$;
Let T be the tree obtained by identifying the roots of T_i and T_j;
Let $\boldsymbol{nb}[\mathtt{a}] := \sum_{\gamma=(\mathtt{a},\mathtt{b},k)\in\Gamma:\mathtt{b}\neq\mathtt{a}\in\Lambda} (\boldsymbol{x}^*_{\mathrm{ex}}(\gamma) - \boldsymbol{f}(\gamma; T)) + 2 \sum_{\gamma=(\mathtt{a},\mathtt{a},k)\in\Gamma} (\boldsymbol{x}^*_{\mathrm{ex}}(\gamma) - \boldsymbol{f}(\gamma; T))$ **for each** $\mathtt{a} \in \Lambda$;
if $\boldsymbol{x}^*_{\mathrm{ex}}(\mathtt{a}) - \boldsymbol{f}_{\mathrm{ex}}(\mathtt{a}; T) \leq \boldsymbol{nb}[\mathtt{a}]$ **for each** $a \in \Lambda$ **then**
$m := k_i + k_j$;
if $w \in \mathrm{W}[\mathtt{a}, 2, m]$ **then** $n_{\boldsymbol{w}}$+= 1
else
$\mathrm{W}[\mathtt{a}, 2, m] := \mathrm{W}[\mathtt{a}, 2, m] \cup \{\boldsymbol{w}\}$; $T_{\boldsymbol{w}} := T$; $n_{\boldsymbol{w}} := 1$
endif
endif
endif
endif
endfor
endfor;
/* It remains to calculate the set $\mathrm{W}^{(0)}_{\mathrm{inl}}(\mathtt{a}, 0, 0)$ and $\mathrm{W}^{(0)}_{\mathrm{inl}+3}(\mathtt{a}, 0, 0)$*/
Let T be a singleton vertex labeled $\mathtt{a}$;
$\mathrm{W}[\mathtt{a}, 0, 0] := \{\boldsymbol{w} = (\mathbf{1}_{\mathtt{a}} + \mathbf{1}_{\mathrm{dg}^+}, \mathbf{0})\}$; $T_{\boldsymbol{w}} := T$; $n_{\boldsymbol{w}} := 1$;

Output $\mathrm{W}[\mathtt{a},d,m]$ as $\mathrm{W}^{(0)}_{\mathrm{end}}(\mathtt{a},d,m)$ (resp., $\mathrm{W}^{(0)}_{\mathrm{inl}}(\mathtt{a},d,m)$ and $\mathrm{W}^{(0)}_{\mathrm{inl+3}}(\mathtt{a},d,m)$),
for each $\boldsymbol{w}\in\mathrm{W}[\mathtt{a},d,m]$, $T_{\boldsymbol{w}}$, and $n_{\boldsymbol{w}}$.

1.3 Computing Weight Vectors of Internal-Subtrees

For an integer $\mathrm{dia}^*\geq 7$, feature vector $x^*=(x^*_{\mathrm{in}},x^*_{\mathrm{ex}})$, integer $n^*_{\mathrm{inl}}=\sum_{\mathtt{a}\in\Lambda}\boldsymbol{x}^*_{\mathrm{in}}(\mathtt{a})$ elements $\mathtt{a}_1,\mathtt{a}_2\in\Lambda$, integers $d_1,d_2\in[1,\mathrm{val}(\mathtt{a}_i)-1]$, $m_i\in[d_i,\mathrm{val}(\mathtt{a}_i)-1]$, $i=1,2$, $h\in[1,\mathrm{dia}^*-\lceil\frac{\mathrm{dia}^*-5}{2}\rceil-1]$ (resp., $h\in[1,\mathrm{dia}^*-7-n^*_{\mathrm{inl}}+\mathrm{dia}^*-2]$) for the case of two leaf 2-branches (resp., three leaf 2-branches), and $\boldsymbol{w}\in\mathrm{W}^{(h)}_{\mathrm{inl}}(\mathtt{a}_1,d_1,m_1,\mathtt{a}_2,d_2,m_2)$, let $\mathcal{T}^{(h)}_{\mathrm{inl}}(\mathtt{a}_1,d_1,m_1,\mathtt{a}_2,d_2,m_2)$ denote the set of sample trees $T_{\boldsymbol{w}}$ and $\mathcal{N}^{(h)}_{\mathrm{inl}}(\mathtt{a}_1,d_1,m_1,\mathtt{a}_2,d_2,m_2)$ denote its size.

For simplicity in our algorithmic notation introduce the set $\mathrm{W}^{(0)}_{\mathrm{inl}}(\mathtt{a}_1,d_1,m_1,\mathtt{a}_1,d_1,m_1)=\mathrm{W}^{(0)}_{\mathrm{inl}}(\mathtt{a}_1,d_1,m_1)$.

Algorithm COMBINEVECTORSETS$(\mathrm{W}_1,\mathtt{a}_1,d_1,m_1,h_1,\mathcal{T}_1,\mathcal{N}_1,\mathrm{W}_2,\mathtt{a}_2,d_2,m_2,0,\mathcal{T}_2,\mathcal{N}_2,m)$
Input: /* Global constant, a vector $\boldsymbol{x}=(\boldsymbol{x}^*_{\mathrm{in}},\boldsymbol{x}^*_{\mathrm{ex}})$ with $\boldsymbol{x}^*_{\mathrm{in}},\boldsymbol{x}^*_{\mathrm{ex}}\in\mathbb{Z}^{\Lambda\cup\Gamma\cup\mathrm{Bc}\cup\mathrm{Dg}}$ */
Sets W_i of vectors $\boldsymbol{z}=(\boldsymbol{z}_{\mathrm{in}},\boldsymbol{z}_{\mathrm{ex}})$ with $\boldsymbol{z}_{\mathrm{in}},\boldsymbol{z}_{\mathrm{ex}}\in\mathbb{Z}^{\Lambda\cup\Gamma\cup\mathrm{Bc}\cup\mathrm{Dg}}$,
elements $\mathtt{a}_i\in\Lambda$ and integers integer $h_1\geq 0$, $d_1\in[0,\mathrm{val}(\mathtt{a}_1)-2]$ (resp., $d_1\in[0,\mathrm{val}(\mathtt{a}_1)-1]$)
if $h_1=0$ (resp., $h_1>0$), $d_2\in[0,\mathrm{val}(\mathtt{a}_2)-2]$, $m_1\in[d_1,\mathrm{val}(\mathtt{a}_1)-2]$ (resp., $m_1\in[d_1,\mathrm{val}(\mathtt{a}_1)-1]$)
if $h_1=0$ (resp., $h_1>0$), $m_2\in[d_2,\mathrm{val}(\mathtt{a}_2)-2]$, such that
for each $\boldsymbol{z}=(\boldsymbol{z}_{\mathrm{in}},\boldsymbol{z}_{\mathrm{ex}})\in\mathrm{W}_i$, $i=1,2$, there exists a bi-rooted tree $T[+2]$,
with $\boldsymbol{f}_{\mathtt{t}}(T[j])=\boldsymbol{z}_{\mathtt{t}}$, $\mathtt{t}\in\{\mathrm{in},\mathrm{ex}\}$, with end vertices u with $\alpha(u)=\mathtt{a}_i$, $i=1,2$;
Sets $\mathcal{T}_i$ of one such sample tree $T_{\boldsymbol{z}}$, and sets $\mathcal{N}_i$ of numbers $n_{\boldsymbol{z}}$ of all possible such trees,
for each $\boldsymbol{z}\in\mathrm{W}_i$, $i=1,2$ and an integer $m\in[1,3]$.
Output: The set W of vectors $\boldsymbol{z}=(\boldsymbol{z}_{\mathrm{in}},\boldsymbol{z}_{\mathrm{ex}})$,
and for each vector $\boldsymbol{z}$ a sample tree $T_{\boldsymbol{z}}$ with
$\boldsymbol{f}_{\mathtt{t}}(T_{\boldsymbol{z}}[+2])=\boldsymbol{z}_{\mathtt{t}}$, $\mathtt{t}\in\{\mathrm{in},\mathrm{ex}\}$, that can be obtained under resource constraint
$\boldsymbol{x}^*=(\boldsymbol{x}^*_{\mathrm{in}},\boldsymbol{x}^*_{\mathrm{ex}})$ by combining vectors $\boldsymbol{z}^1=(\boldsymbol{z}^1_{\mathrm{in}},\boldsymbol{z}^1_{\mathrm{ex}})$ and $\boldsymbol{z}^2=(\boldsymbol{z}^2_{\mathrm{in}},\boldsymbol{z}^2_{\mathrm{ex}})$, $\boldsymbol{z}^i\in\mathrm{W}_i$, $i=1,2$,
and for each vector $\boldsymbol{z}$ the number $n_{\boldsymbol{z}}$ of possible internal trees
that satisfy the weight vectors in the set W, where $\boldsymbol{z}$, a sample tree $T_{\boldsymbol{z}}$ and $n_{\boldsymbol{z}}$ are stored in a trie.
$\mathrm{W}:=\emptyset$;
for each $\boldsymbol{w}^1=(\boldsymbol{w}^1_{\mathrm{in}},\boldsymbol{w}^1_{\mathrm{ex}})\in\mathrm{W}_1$, $\boldsymbol{w}^2=(\boldsymbol{w}^2_{\mathrm{in}},\boldsymbol{w}^2_{\mathrm{ex}})\in\mathrm{W}_2$ **do**
if
- $\gamma=(\mathtt{a}_1,\mathtt{a}_2,m)\in\Gamma$,
- $\mu=(d_1+2,d_2+2,m)\in\mathrm{Bc}$ (resp., $\mu=(d_1+1,d_2+2,m)\in\mathrm{Bc}$),
if $h_1=0$ (resp., $h_1>0$)
- $m+m_1+1\leq\mathrm{val}(\mathtt{a}_1)$ (resp., $m+m_1\leq\mathrm{val}(\mathtt{a}_1)$) if $h_1=0$ (resp., $h_1>0$)
- $m+m_2+1\leq\mathrm{val}(\mathtt{a}_2)$ **do**

$\boldsymbol{w}_{\mathrm{ex}}:=\boldsymbol{w}^1_{\mathrm{ex}}+\boldsymbol{w}^2_{\mathrm{ex}}$; $\boldsymbol{w}_{\mathrm{in}}:=\boldsymbol{w}^1_{\mathrm{in}}+\boldsymbol{w}^2_{\mathrm{in}}+\mathbf{1}_\gamma+\mathbf{1}_\mu$;
if $\boldsymbol{w}_{\mathrm{in}}\leq\boldsymbol{x}^*_{\mathrm{in}}$ **and** $\boldsymbol{w}_{\mathrm{ex}}\leq\boldsymbol{x}^*_{\mathrm{ex}}$ **then**
if $\boldsymbol{w}=(\boldsymbol{w}_{\mathrm{in}},\boldsymbol{w}_{\mathrm{ex}})\in\mathrm{W}$ **then** $n_{\boldsymbol{w}}=n_{\boldsymbol{w}}+n_{\boldsymbol{w}^1}\cdot n_{\boldsymbol{w}^2}$
else
Let T be the tree obtained by joining the roots of $T_{\boldsymbol{w}^1}$ and $T_{\boldsymbol{w}^2}$ with labels $\mathtt{a}_1$ and $\mathtt{a}_2$,

respectively, by an edge of multiplicity m;
W $:=$ W $\cup \{\boldsymbol{w}\}$; $T_{\boldsymbol{w}} := T$; $n_{\boldsymbol{w}} := n_{\boldsymbol{w}^1} \cdot n_{\boldsymbol{w}^2}$
end if
end if
end for;
Output W and for each $\boldsymbol{w} \in$ W, $T_{\boldsymbol{w}}$ and $n_{\boldsymbol{w}}$.

For simplicity, we denote by $\mathrm{W}_1 \oplus \mathrm{W}_2$ the output of calling Algorithm CombineVectorSets($\mathrm{W}_1, \mathtt{a}_1, d_1, m_1, i, \mathcal{T}_1, \mathcal{N}_1, \mathrm{W}_2, \mathtt{a}_2, d_2, m_2, \mathcal{T}_2, \mathcal{N}_2, m)$.

Algorithm ComputeInternalTreeSequential$(\mathtt{a}, d_{\mathtt{a}}, m_{\mathtt{a}}, \mathtt{b}, d_{\mathtt{b}}, m_{\mathtt{a}}, h)$
Input: Elements $\mathtt{a}, \mathtt{b} \in \Lambda$, integers $h \geq 1$, $d_{\mathtt{a}} \in [1, \mathrm{val}(\mathtt{a}) - 1]$, $m_{\mathtt{a}} \in [d_{\mathtt{a}}, \mathrm{val}(\mathtt{a}) - 1]$
$d_{\mathtt{b}} \in [1, \mathrm{val}(\mathtt{b}) - 1]$, $m_{\mathtt{b}} \in [d_{\mathtt{b}}, \mathrm{val}(\mathtt{b}) - 2]$.
/* Global data: A vector $\boldsymbol{x} = (\boldsymbol{x}^*_{\mathrm{in}}, \boldsymbol{x}^*_{\mathrm{ex}})$ with $\boldsymbol{x}^*_{\mathrm{in}}, \boldsymbol{x}^*_{\mathrm{ex}} \in \mathbb{Z}^{\Lambda \cup \Gamma \cup \mathrm{Bc} \cup \mathrm{Dg}}$,
the collection of sets $\mathrm{W}^{(0)}_{\mathrm{inl}}(\mathtt{a}', d', m', \mathtt{a}', d', m')$, with their collections
$\mathcal{T}^{(0)}_{\mathrm{inl}}(\mathtt{a}', d', m', \mathtt{a}', d', m')$ of representative trees and
$\mathcal{N}^{(0)}_{\mathrm{inl}}(\mathtt{a}', d', m', \mathtt{a}', d', m')$ of number of trees satisfying each vector, $\mathtt{a}' \in \Lambda, d' \in [0, \mathrm{val}(\mathtt{a}') - 2]$,
$m' \in [d', \mathrm{val}(\mathtt{a}') - 2]$. */
Output: The set $\mathrm{W}^{(h)}_{\mathrm{inl}}(\mathtt{a}, d_{\mathtt{a}}, m_{\mathtt{a}}, \mathtt{b}, d_{\mathtt{b}}, m_{\mathtt{b}})$,
sets $\mathcal{T}^{(h)}_{\mathrm{inl}}(\mathtt{a}, d_{\mathtt{a}}, m_{\mathtt{a}}, \mathtt{b}, d_{\mathtt{b}}, m_{\mathtt{b}})$ and $\mathcal{N}^{(h)}_{\mathrm{inl}}(\mathtt{a}, d_{\mathtt{a}}, m_{\mathtt{a}}, \mathtt{b}, d_{\mathtt{b}}, m_{\mathtt{b}})$
of representative trees and number of trees that satisfy each vector
$\boldsymbol{w} \in \mathrm{W}^{(h)}_{\mathrm{inl}}(\mathtt{a}, d_{\mathtt{a}}, m_{\mathtt{a}}, \mathtt{b}, d_{\mathtt{b}}, m_{\mathtt{b}})$, where vectors $\boldsymbol{w}$ and a sample tree $T_{\boldsymbol{w}}$ and the number $n_{\boldsymbol{w}}$ of trees with vector $\boldsymbol{w}$ are stored in a trie.
$\mathrm{W}[\mathtt{a}_1, d_1, m_1, \mathtt{a}_2, d_2, m_2, j] := \emptyset$ **for each** $j \in [0, h]$ $\mathtt{a}_i \in \Lambda$, $d_1 \in [0, \mathrm{val}(\mathtt{a}_1) - 2]$
(resp., $d_1 \in [0, \mathrm{val}(\mathtt{a}_1) - 1]$) if $j = 0$ (resp., $j > 0$), $d_2 \in [0, \mathrm{val}(\mathtt{a}_2) - 2]$, $m_1 \in [d_1, \mathrm{val}(\mathtt{a}_1) - 2]$
(resp., $m_1 \in [d_1, \mathrm{val}(\mathtt{a}_1) - 1]$) if $j = 0$ (resp., $j > 0$), $m_2 \in [d_2, \mathrm{val}(\mathtt{a}_2) - 2]$;
$\mathrm{W}[\mathtt{a}_1, d_1, m_1, \mathtt{a}_1, d_1, m_1, 0] := \mathrm{W}^{(0)}_{\mathrm{inl}}(\mathtt{a}_1, d_1, m_1, \mathtt{a}_1, d_1, m_1)$ **for each** $\mathtt{a}_1 \in \Lambda$,
$d_1 \in [0, \mathrm{val}(\mathtt{a}_1) - 2]$, $m_1 \in [0, \mathrm{val}(\mathtt{a}_1) - 2]$;
for each $i \in [1, h]$ **do**
for each triplet $(\mathtt{a}', d'_{\mathtt{a}}, m'_{\mathtt{a}})$ **do**
for each triplet $(\mathtt{b}', d'_{\mathtt{b}}, m'_{\mathtt{b}})$ **do**
for each triplet $(\mathtt{a}'', d''_{\mathtt{a}}, m''_{\mathtt{a}})$ **do**
for each $m^* \in [1, 3]$ **do**
if $i = 1$ **then**
$\mathrm{W} := \mathrm{W}[\mathtt{a}', d'_{\mathtt{a}} - 1, m'_{\mathtt{a}} - m^*, \mathtt{a}'', d''_{\mathtt{a}} - 1, m''_{\mathtt{a}} - m^*, i - 1] \oplus$
$\mathrm{W}[\mathtt{b}', d'_{\mathtt{b}} - 1, m'_{\mathtt{b}} - m^*, \mathtt{b}', d'_{\mathtt{b}} - 1, m'_{\mathtt{b}} - m^*, 0]$;
else
$\mathrm{W} := \mathrm{W}[\mathtt{a}', d'_{\mathtt{a}}, m'_{\mathtt{a}}, \mathtt{a}'', d''_{\mathtt{a}}, m''_{\mathtt{a}}, i - m^*] \oplus$
$\mathrm{W}[\mathtt{b}', d'_{\mathtt{b}} - 1, m'_{\mathtt{b}} - m^*, \mathtt{b}', d'_{\mathtt{b}} - 1, m'_{\mathtt{b}} - m^*, 0]$;
end if;
$\mathrm{W}[\mathtt{a}', d'_{\mathtt{a}}, m'_{\mathtt{a}}, \mathtt{b}', d'_{\mathtt{b}}, m'_{\mathtt{b}}, i] := \mathrm{W}[\mathtt{a}', d'_{\mathtt{a}}, m'_{\mathtt{a}}, \mathtt{b}', d'_{\mathtt{b}}, m'_{\mathtt{b}}, i] \cup \mathrm{W}$
end for

end for
end for
end for
end for;
Output $\mathrm{W}[\mathtt{a}, d_{\mathtt{a}}, m_{\mathtt{a}}, \mathtt{b}, d_{\mathtt{b}}, m_{\mathtt{b}}, h]$ as $\mathrm{W}^{(h)}_{\mathrm{inl}}(\mathtt{a}, d_{\mathtt{a}}, m_{\mathtt{a}}, \mathtt{b}, d_{\mathtt{b}}, m_{\mathtt{b}})$ for $\boldsymbol{w} \in \mathrm{W}[\mathtt{a}, d_{\mathtt{a}}, m_{\mathtt{a}}, \mathtt{b}, d_{\mathtt{b}}, m_{\mathtt{b}}, h]$, $T_{\boldsymbol{w}}$ and $n_{\boldsymbol{w}}$.

1.4 Computing Weight Vectors of End-Subtrees with one and two fictitious edges

We here give an outline of procedures to generate the sets of frequency vector of bi-rooted trees with one and two fictitious edges.

Computing vectors of end-subtrees with one fictitious edge
For an integer $\delta \geq 1$, element $\mathtt{a} \in \Lambda$, integers $d_{\mathtt{a}} \in [1, \mathrm{val}(\mathtt{a}) - 1]$, and $m_{\mathtt{a}} \in [d_{\mathtt{a}}, \mathrm{val}(\mathtt{a}) - 1]$ we give a procedure to compute the set $\mathrm{W}^{(\delta)}_{\mathrm{end}}(\mathtt{a}, d_{\mathtt{a}}, m_{\mathtt{a}})$.

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

Input: Element $\mathtt{a} \in \Lambda$, integer $d \in [1, \mathrm{val}(a) - 1]$, $m \in [d, \mathrm{val}(a) - 1]$, $\delta \geq 1$.
/* Global data: A vector $\boldsymbol{x}^* = (\boldsymbol{x}^*_{\mathrm{in}}, \boldsymbol{x}^*_{\mathrm{ex}})$ with $\boldsymbol{x}^*_{\mathrm{in}}, \boldsymbol{x}^*_{\mathrm{ex}} \in \mathbb{Z}^{\Lambda \cup \Gamma \cup \mathrm{Bc} \cup \mathrm{Dg}}$, the collection $\mathcal{W}^{(0)}_{\mathrm{end}}$ of vector sets $\mathrm{W}^{(0)}_{\mathrm{end}}(\mathtt{b}, d_{\mathtt{b}}, m_{\mathtt{b}})$, $\mathtt{b} \in \Lambda$, $d_{\mathtt{b}} \in [1, \mathrm{val}(\mathtt{b}) - 1]$, $m_{\mathtt{b}} \in [d_{\mathtt{b}}, \mathrm{val}(\mathtt{b}) - 1]$ $\mathcal{W}^{(\delta-1)}_{\mathrm{inl}}$ of vector sets $\mathrm{W}^{(\delta-1)}_{\mathrm{inl}}(\mathtt{a}_1, d_1, m_1, \mathtt{a}_2, d_2, m_1)$, $\mathtt{a}_1, \mathtt{a}_2 \in \Lambda$, $d_i \in [1, \mathrm{val}(\mathtt{a}_i) - 1]$ (resp., $d_i \in [0, \mathrm{val}(\mathtt{a}_i) - 2]$), $i = 1, 2$ if $\delta > 1$ (resp., $\delta = 1$) */
Output: The set $\mathrm{W}^{(\delta)}_{\mathrm{end}}(\mathtt{a}, d, m)$, where we store each vector $\boldsymbol{w} \in \mathrm{W}^{(\delta)}_{\mathrm{end}}(\mathtt{a}, d, m)$, a sample tree $T_{\boldsymbol{w}}$ and the 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 $(\mathtt{a}', d'_{\mathtt{a}}, m'_{\mathtt{a}})$ **do**
for each $\boldsymbol{w}^{\mathtt{b}} = (\boldsymbol{w}^{\mathtt{b}}_{\mathrm{in}}, \boldsymbol{w}^{\mathtt{b}}_{\mathrm{ex}}) \in \mathrm{W}^{(0)}_{\mathrm{end}}(\mathtt{b}, d_{\mathtt{b}}, m_{\mathtt{b}})$, **do**
for each $m' \in [1, 3]$ such that
- $\gamma = (\mathtt{a}', \mathtt{b}, m') \in \Gamma$,
- $\mu = (d'_{\mathtt{a}} + 1, d_{\mathtt{b}} + 1, m') \in \mathrm{Bc}$ (resp., $\mu = (d'_{\mathtt{a}} + 2, d_{\mathtt{b}} + 1, m') \in \mathrm{Bc}$) if $\delta > 1$ (resp., $\delta = 1$) and
- $m' + m'_{\mathtt{a}} \leq \mathrm{val}(\mathtt{a}')$ (resp., $m' + m'_{\mathtt{a}} + 1 \leq \mathrm{val}(\mathtt{a}')$, $m' + m'_{\mathtt{a}} = m$) if $\delta > 1$ (resp., $\delta = 1$) and $m' + m_{\mathtt{b}} \leq \mathrm{val}(\mathtt{b})$ **do**
for each $\boldsymbol{w}^{\mathtt{a}} = (\boldsymbol{w}^{\mathtt{a}}_{\mathrm{in}}, \boldsymbol{w}^{\mathtt{a}}_{\mathrm{ex}}) \in \mathrm{W}^{(\delta-1)}_{\mathrm{inl}}(\mathtt{a}', d'_{\mathtt{a}}, m'_{\mathtt{a}}, \mathtt{a}, d, m)$ (resp., $\boldsymbol{w}^{\mathtt{a}} = (\boldsymbol{w}^{\mathtt{a}}_{\mathrm{in}}, \boldsymbol{w}^{\mathtt{a}}_{\mathrm{ex}}) \in$ '$\mathrm{W}^{(\delta-1)}_{\mathrm{inl}}(\mathtt{a}', d-1, m'_{\mathtt{a}}, \mathtt{a}, d-1, m'_{a})$) if $\delta > 1$ (resp., $\delta = 1$) **do**
$\boldsymbol{w}_{\mathrm{in}} := \boldsymbol{w}^{\mathtt{a}}_{\mathrm{in}} + \boldsymbol{w}^{\mathtt{b}}_{\mathrm{in}} + \mathbf{1}_{\mu} + \mathbf{1}_{\gamma}$;
$\boldsymbol{w}_{\mathrm{ex}} := \boldsymbol{w}^{\mathtt{a}}_{\mathrm{ex}} + \boldsymbol{w}^{\mathtt{b}}_{\mathrm{ex}}$;
if $\boldsymbol{w} = (\boldsymbol{w}_{\mathrm{in}}, \boldsymbol{w}_{\mathrm{ex}}) \in \mathrm{W}$ **then** $n_{\boldsymbol{w}} = n_{\boldsymbol{w}} + n_{\boldsymbol{w}^{\mathtt{a}}} \cdot n_{\boldsymbol{w}^{\mathtt{b}}}$
else

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;
$\mathrm{W} := \mathrm{W} \cup \{(\boldsymbol{w}_{\mathrm{in}}, \boldsymbol{w}_{\mathrm{ex}})\}$; $T_{\boldsymbol{w}} := T$; $n_{\boldsymbol{w}} := n_{\boldsymbol{w}^{\mathtt{a}}} \cdot n_{\boldsymbol{w}^{\mathtt{b}}}$
end if
end for
end for
end for
end for
end for;
Output W as $\mathrm{W}^{(\delta)}_{\mathrm{end}}(\mathtt{a}, d, m)$, and for each $\boldsymbol{w} \in \mathrm{W}$, $T_{\boldsymbol{w}}$ and $n_{\boldsymbol{w}}$.

Computing vectors of end-subtrees with two fictitious edge
For an integer $\delta \geq 2$, element $\mathtt{a} \in \Lambda$, integers $d_{\mathtt{a}} \in [1, \mathrm{val}(\mathtt{a}) - 2]$, and $m_{\mathtt{a}} \in [d_{\mathtt{a}}, \mathrm{val}(\mathtt{a}) - 1]$ we give a procedure to compute the set $\mathrm{W}^{(\delta)}_{\mathrm{end+2}}(\mathtt{a}, d_{\mathtt{a}}, m_{\mathtt{a}})$.

ComputeEndSubtreeTwo$(\mathtt{a}, d, m, \delta)$

Input: Element $\mathtt{a} \in \Lambda$, integer $d \in [1, \mathrm{val}(a) - 2]$, $m \in [d, \mathrm{val}(a) - 2]$, $\delta \geq 2$.
/* Global data: A vector $\boldsymbol{x}^* = (\boldsymbol{x}^*_{\mathrm{in}}, \boldsymbol{x}^*_{\mathrm{ex}})$ with $\boldsymbol{x}^*_{\mathrm{in}}, \boldsymbol{x}^*_{\mathrm{ex}} \in \mathbb{Z}^{\Lambda \cup \Gamma \cup \mathrm{Bc} \cup \mathrm{Dg}}$, the collection
$\mathcal{W}^{(0)}_{\mathrm{inl+3}}$ of vector sets $\mathrm{W}^{(0)}_{\mathrm{inl+3}}(\mathtt{a}, d-1, m_{\mathtt{a}})$, $m_{\mathtt{a}} \in [d-1, \mathrm{val}(\mathtt{a}) - 3]$
$\mathcal{W}^{(\delta-1)}_{\mathrm{end}}$ of vector sets $\mathrm{W}^{(\delta-1)}_{\mathrm{end}}(\mathtt{a}_1, d_1, m_1)$, $\mathtt{a}_1 \in \Lambda$, $d_1 \in [1, \mathrm{val}(\mathtt{a}_1) - 1]$ */
Output: The set $\mathrm{W}^{(\delta)}_{\mathrm{end+2}}(\mathtt{a}, d, m)$, where we store each vector $\boldsymbol{w} \in \mathrm{W}^{(\delta)}_{\mathrm{end+2}}(\mathtt{a}, d, m)$, a sample tree $T_{\boldsymbol{w}}$ 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 $\boldsymbol{w}^{\mathtt{b}} = (\boldsymbol{w}^{\mathtt{b}}_{\mathrm{in}}, \boldsymbol{w}^{\mathtt{b}}_{\mathrm{ex}}) \in \mathrm{W}^{(\delta-1)}_{\mathrm{end}}(\mathtt{b}, d_{\mathtt{b}}, m_{\mathtt{b}})$, **do**
for each $m' \in [1, 3]$ such that
- $\gamma = (\mathtt{a}, \mathtt{b}, m') \in \Gamma$,
- $\mu = (d+2, d_{\mathtt{b}}+1, m') \in \mathrm{Bc}$ and
- $m_{\mathtt{a}} + m' = m, m_{\mathtt{a}} + m' + 2 \leq \mathrm{val}(\mathtt{a})$ and $m' + m_{\mathtt{b}} \leq \mathrm{val}(\mathtt{b})$ **do**
for each $\boldsymbol{w}^{\mathtt{a}} = (\boldsymbol{w}^{\mathtt{a}}_{\mathrm{in}}, \boldsymbol{w}^{\mathtt{a}}_{\mathrm{ex}}) \in \mathrm{W}^{(0)}_{\mathrm{inl+3}}(\mathtt{a}, d-1, m_{\mathtt{a}})$ **do**
$\boldsymbol{w}_{\mathrm{in}} := \boldsymbol{w}^{\mathtt{a}}_{\mathrm{in}} + \boldsymbol{w}^{\mathtt{b}}_{\mathrm{in}} + \mathbf{1}_{\mu} + \mathbf{1}_{\gamma}$;
$\boldsymbol{w}_{\mathrm{ex}} := \boldsymbol{w}^{\mathtt{a}}_{\mathrm{ex}} + \boldsymbol{w}^{\mathtt{b}}_{\mathrm{ex}}$;
if $\boldsymbol{w} = (\boldsymbol{w}_{\mathrm{in}}, \boldsymbol{w}_{\mathrm{ex}}) \in \mathrm{W}$ **then** $n_{\boldsymbol{w}} = n_{\boldsymbol{w}} + n_{\boldsymbol{w}^{\mathtt{a}}} \cdot n_{\boldsymbol{w}^{\mathtt{b}}}$
else
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;
$\mathrm{W} := \mathrm{W} \cup \{(\boldsymbol{w}_{\mathrm{in}}, \boldsymbol{w}_{\mathrm{ex}})\}$; $T_{\boldsymbol{w}} := T$; $n_{\boldsymbol{w}} := n_{\boldsymbol{w}^{\mathtt{a}}} \cdot n_{\boldsymbol{w}^{\mathtt{b}}}$
end if
end for
end for
end for
end for

end for;
Output W as $\mathrm{W}^{(\delta)}_{\mathrm{end}+2}(\mathtt{a}, d, m)$, and for each $\boldsymbol{w} \in \mathrm{W}$, $T_{\boldsymbol{w}}$ and $n_{\boldsymbol{w}}$.

1.5 Computing Weight Vectors of Main-Subtrees

Consider the case of three leaf 2-branches. For an element $\mathtt{a} \in \Lambda$, and integers $d \in [2, \mathrm{val}(\mathtt{a}) - 1]$, $m \in [d, \mathrm{val}(\mathtt{a}) - 1]$, and $\delta \geq 1$ we give a procedure to compute the set $\mathrm{W}^{(\delta+1)}_{\mathrm{main}}(\mathtt{a}, d, m)$.

ComputeMainTree$(\mathtt{a}, d, m, \delta)$

Input: Element $\mathtt{a} \in \Lambda$, integer $d \in [2, \mathrm{val}(a) - 1]$, $m \in [d, \mathrm{val}(a) - 1]$, $\delta \geq 1$.
/* Global data: An integer dia*, a vector $\boldsymbol{x}^* = (\boldsymbol{x}^*_{\mathrm{in}}, \boldsymbol{x}^*_{\mathrm{ex}})$ with $\boldsymbol{x}^*_{\mathrm{in}}, \boldsymbol{x}^*_{\mathrm{ex}} \in \mathbb{Z}^{\Lambda \cup \Gamma \cup \mathrm{Bc} \cup \mathrm{Dg}}$, the collection
$\mathcal{W}^{(\delta+1)}_{\mathrm{end}+2}$ of vector sets $\mathrm{W}^{(\delta+1)}_{\mathrm{end}+2}(\mathtt{a}, d-1, m_{\mathtt{a}})$, $m_{\mathtt{a}} \in [d-1, \mathrm{val}(\mathtt{a}) - 2]$
$\mathcal{W}^{(\delta')}_{\mathrm{end}}$ of vector sets $\mathrm{W}^{(\delta')}_{\mathrm{end}}(\mathtt{a}_1, d_1, m_1)$, $\mathtt{a}_1 \in \Lambda$, $d_1 \in [1, \mathrm{val}(\mathtt{a}_1) - 1]$ such that $\delta + \delta' + 2 = \mathrm{dia}^* - 4$. */
Output: The set $\mathrm{W}^{(\delta+1)}_{\mathrm{main}}(\mathtt{a}, d, m)$, where we store each vector $\boldsymbol{w} \in \mathrm{W}^{(\delta+1)}_{\mathrm{main}}(\mathtt{a}, d, m)$, a sample tree $T_{\boldsymbol{w}}$ and number $n_{\boldsymbol{w}}$ of trees with vector $\boldsymbol{w}$ in a trie.
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 $\boldsymbol{w}^{\mathtt{b}} = (\boldsymbol{w}^{\mathtt{b}}_{\mathrm{in}}, \boldsymbol{w}^{\mathtt{b}}_{\mathrm{ex}}) \in \mathrm{W}^{(\delta')}_{\mathrm{end}}(\mathtt{b}, d_{\mathtt{b}}, m_{\mathtt{b}})$, **do**
      for each $m' \in [1, 2]$ such that
        - $\gamma = (\mathtt{a}, \mathtt{b}, m') \in \Gamma$,
        - $\mu = (d+1, d_{\mathtt{b}}+1, m') \in \mathrm{Bc}$ 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 $\boldsymbol{w}^{\mathtt{a}} = (\boldsymbol{w}^{\mathtt{a}}_{\mathrm{in}}, \boldsymbol{w}^{\mathtt{a}}_{\mathrm{ex}}) \in \mathrm{W}^{(\delta+1)}_{\mathrm{end}+2}(\mathtt{a}, d-1, m_{\mathtt{a}})$ **do**
          $\boldsymbol{w}_{\mathrm{in}} := \boldsymbol{w}^{\mathtt{a}}_{\mathrm{in}} + \boldsymbol{w}^{\mathtt{b}}_{\mathrm{in}} + \mathbf{1}_{\mu} + \mathbf{1}_{\gamma}$;
          $\boldsymbol{w}_{\mathrm{ex}} := \boldsymbol{w}^{\mathtt{a}}_{\mathrm{ex}} + \boldsymbol{w}^{\mathtt{b}}_{\mathrm{ex}}$;
          if $\boldsymbol{w} = (\boldsymbol{w}_{\mathrm{in}}, \boldsymbol{w}_{\mathrm{ex}}) \in \mathrm{W}$ **then** $n_{\boldsymbol{w}} = n_{\boldsymbol{w}} + n_{\boldsymbol{w}^{\mathtt{a}}} \cdot n_{\boldsymbol{w}^{\mathtt{b}}}$
          else
            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;
            $\mathrm{W} := \mathrm{W} \cup \{(\boldsymbol{w}_{\mathrm{in}}, \boldsymbol{w}_{\mathrm{ex}})\}$; $T_{\boldsymbol{w}} := T$; $n_{\boldsymbol{w}} := n_{\boldsymbol{w}^{\mathtt{a}}} \cdot n_{\boldsymbol{w}^{\mathtt{b}}}$
          end if
        end for
      end for
    end for
  end for
end for;
Output W as $\mathrm{W}^{(\delta+1)}_{\mathrm{main}}(\mathtt{a}, d, m)$, and for each $\boldsymbol{w} \in \mathrm{W}$, $T_{\boldsymbol{w}}$ and $n_{\boldsymbol{w}}$.

1.6 Computing Feasible Vector Pairs

We give a procedure to compute feasible vector pairs for the cases of two and three leaf 2-branches.

For the case of two leaf 2-branches, we take $\delta_1 = \lfloor \frac{\mathrm{dia}^*-5}{2} \rfloor$ and $\delta_2 = \mathrm{dia}^* - 5 - \delta_1 = \lceil \frac{\mathrm{dia}^*-5}{2} \rceil$. and compute feasible pair of vectors $\boldsymbol{w}^i = (\boldsymbol{w}^i_{\mathrm{in}}, \boldsymbol{w}^i_{\mathrm{ex}}) \in \mathrm{W}^{(\delta_i)}_{\mathrm{end}}(\mathtt{a}_i, d_i, m_i)$, $\mathtt{a}_i \in \Lambda$, $d_i \in [1, \mathrm{val}(\mathtt{a}_i) - 1]$, $m_i \in [d_i, \mathrm{val}(\mathtt{a}_i) - 1]$, $i = 1, 2$.

For the case of three leaf 2-branches, we take $\delta_1 \in \lceil \mathrm{dia}^*/2 \rceil - 3, \mathrm{dia}^* - 6 - \delta_3]$, $\mathtt{a}_i \in \Lambda$, and $\delta_3 = n^*_{\mathrm{inl}} - \mathrm{dia}^* + 2$ and compute feasible pair of vectors $\boldsymbol{w}^1 = (\boldsymbol{w}^1_{\mathrm{in}}, \boldsymbol{w}^1_{\mathrm{ex}}) \in \mathrm{W}^{(\delta_1+1)}_{\mathrm{main}}(\mathtt{a}_1, d_1, m_1)$, and $\boldsymbol{w}^2 = (\boldsymbol{w}^2_{\mathrm{in}}, \boldsymbol{w}^2_{\mathrm{ex}}) \in \mathrm{W}^{(\delta_3)}_{\mathrm{end}}(\mathtt{a}_2, d_2, m_2)$, $d_i \in [1, \mathrm{val}(\mathtt{a}_i) - 1]$, $m_i \in [d_i, \mathrm{val}(\mathtt{a}_i) - 1]$, $i = 1, 2$.

Define the (γ, μ)-*complement vector* $\overline{\boldsymbol{z}} = (\overline{\boldsymbol{z}}_{\mathrm{in}}, \overline{\boldsymbol{z}}_{\mathrm{ex}})$ of a vector $\boldsymbol{z} = (\boldsymbol{z}_{\mathrm{in}}, \boldsymbol{z}_{\mathrm{ex}}) \in \mathrm{W}^{(\delta)}_{\mathrm{end}}(\mathtt{a}, d, m)$ (resp., $\boldsymbol{z} = (\boldsymbol{z}_{\mathrm{in}}, \boldsymbol{z}_{\mathrm{ex}}) \in \mathrm{W}^{(\delta+1)}_{\mathrm{main}}(\mathtt{a}, d, m)$) to be such that $\overline{\boldsymbol{z}_{\mathrm{in}}} = \boldsymbol{x}^*_{\mathrm{in}} - \mathbf{1}_\gamma - \mathbf{1}_\mu - \boldsymbol{z}_{\mathrm{in}}$ and $\overline{\boldsymbol{z}_{\mathrm{ex}}} = \boldsymbol{x}^*_{\mathrm{ex}} - \boldsymbol{z}_{\mathrm{ex}}$.

Algorithm COMBINE(global data: $\boldsymbol{x}^* = (\boldsymbol{x}^*_{\mathrm{in}}, \boldsymbol{x}^*_{\mathrm{ex}})$)
Input: Two sets W_1 and W_2 such that $\mathrm{W}_1(\mathtt{a}_1, d_1, m_1) = \mathrm{W}^{(\delta_1)}_{\mathrm{end}}(\mathtt{a}_1, d_1, m_1)$ and
$\mathrm{W}_2(\mathtt{a}_2, d_2, m_2) = \mathrm{W}^{(\delta_2)}_{\mathrm{end}}(\mathtt{a}_2, d_2, m_2)$ (resp., $\mathrm{W}_1(\mathtt{a}_1, d_1, m_1) = \mathrm{W}^{(\delta_1+1)}_{\mathrm{main}}(\mathtt{a}_1, d_1, m_1)$ and
$\mathrm{W}_2(\mathtt{a}_2, d_2, m_2) = \mathrm{W}^{(\delta_3)}_{\mathrm{end}}(\mathtt{a}_2, d_2, m_2)$
for the case of two leaf 2-branches (resp., three leaf 2-branches), where we assume that all
vectors $\boldsymbol{z} = (\boldsymbol{z}_{\mathrm{in}}, \boldsymbol{z}_{\mathrm{ex}})$ with $\boldsymbol{z}_{\mathrm{in}}, \boldsymbol{z}_{\mathrm{ex}} \in \mathbb{Z}^{\Lambda \cup \Gamma \cup \mathrm{Bc} \cup \mathrm{Dg}}$ in each set $\mathrm{W}_i(\mathtt{a}_i, d_i, m_i), i = 1, 2$
have been sorted in a lexicographical order.
Output: All feasible pairs $(\boldsymbol{z}_1, \boldsymbol{z}_2)$ of vectors,
for each pair a tree that satisfies the combined vector,
and a lower number ℓ on the total number of trees that satisfy all
feasible pairs of vectors.
$\ell := 0$;
for each pair of $\gamma = (\mathtt{a}_1, \mathtt{a}_2, k) \in \Gamma$ and $\mu = (d_1 + 1, d_2 + 1, k) \in \mathrm{Bc}$ with
$m_i + k \leq \mathrm{val}(\mathtt{a}_i)$, $i = 1, 2$ **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, μ)-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 $L_{\gamma,\mu}$ of vectors in both lists (as a multiset);
Trace the list $L_{\gamma,\mu}$ 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 bond configuration γ;
/* Execute the next if-condition for the case of two leaf 2-branches */
if $\delta_1 = \delta_2$ and $(\mathtt{a}_1, d_1, m_1) = (\mathtt{a}_2, d_2, m_2)$ **then**
$\ell := \ell + \lceil (n_{\boldsymbol{z}^1} \cdot n_{\overline{\boldsymbol{z}^2}})/2 \rceil$
else
$\ell := \ell + n_{\boldsymbol{z}^1} \cdot n_{\overline{\boldsymbol{z}^2}}$
endif;
/* Execute the next for the case of three leaf 2-branches */
$\delta := \mathrm{dia}^* - 4 - \delta_1 - 1 - 1$;
if $\delta = \delta_3$ **then**
if $\delta_1 = \delta$ **then**
$\ell := \ell + \lceil (n_{\boldsymbol{z}^1} \cdot n_{\overline{\boldsymbol{z}^2}})/6 \rceil$
else
$\ell := \ell + \lceil (n_{\boldsymbol{z}^1} \cdot n_{\overline{\boldsymbol{z}^2}})/2 \rceil$

endif
else if $\delta_1 - 1 = \delta$ **then**
$\ell := \ell + \lceil (n_{\boldsymbol{z}^1} \cdot n_{\overline{\boldsymbol{z}^2}})/2 \rceil$
else
$\ell := \ell + n_{\boldsymbol{z}^1} \cdot n_{\overline{\boldsymbol{z}^2}}$
endif
endfor;
Output ℓ.

1.7 A Complete Algorithm for the Case of Two Leaf 2-Branch number

We briefly summarize how to use the procedures described thus far to obtain an algorithm. Our global constants are a resource vector $\boldsymbol{x}^* = (\boldsymbol{x}^*_{\rm in}, \boldsymbol{x}^*_{\rm ex})$ with $\boldsymbol{x}^*_{\rm in}, \boldsymbol{x}^*_{\rm ex} \in \mathbb{Z}^{\Lambda\cup\Gamma\cup{\rm Bc}\cup{\rm Dg}}$ and an integer dia*.

TwoLeafBranchCompleteAlgorithm(Global constants: $\boldsymbol{x}^* = (\boldsymbol{x}^*_{\rm in}, \boldsymbol{x}^*_{\rm ex}), {\rm dia}^*$)

$\delta_1 := \lfloor ({\rm dia}^* - 5)/2 \rfloor$, $\delta_2 := \lceil ({\rm dia}^* - 5)/2 \rceil$;
Compute the sets $W^{(0)}_{\rm end}(\mathtt{a}, d, m)$ **for each** $\mathtt{a} \in \Lambda$, $d \in [1, {\rm val}(\mathtt{a}) - 1]$, $m \in [d, {\rm val}(\mathtt{a}) - 1]$;
Compute the sets $W^{(0)}_{\rm inl}(\mathtt{a}, d, m)$ **for each** $\mathtt{a} \in \Lambda$, $d \in [0, {\rm val}(\mathtt{a}) - 2]$, $m \in [d, {\rm val}(\mathtt{a}) - 2]$;
for each tuple $(\mathtt{a}_1, d_1, m_1, \mathtt{a}_2, d_2, m_2)$ with $\mathtt{a}_1, \mathtt{a}_2 \in \Lambda$, $d_i \in [1, {\rm val}(\mathtt{a}_i) - 1]$, $m_i \in [d_i, {\rm val}(\mathtt{a}_i) - 1]$ **do**
  Compute the sets $W^{(h)}_{\rm inl}(\mathtt{a}_1, d_1, m_1, \mathtt{a}_2, d_2, m_2)$, $h = \delta_1 - 1, \delta_2 - 1$
end for;
Compute the sets $W^{(h)}_{\rm end}(\mathtt{a}, d, m)$ **for each** $\mathtt{a} \in \Lambda$, $d \in [1, {\rm val}(\mathtt{a}) - 1]$, $m \in [d, {\rm val}(\mathtt{a}) - 1]$, $h = \delta_1, \delta_2$;
for each two triplets $(\mathtt{a}_i, d_i, m_i)$ with $\mathtt{a}_i \in \Lambda$, $d_i \in [1, {\rm val}(\mathtt{a}_i) - 1]$, $m_i \in [d_i, {\rm val}(\mathtt{a}_i) - 1]$ **do**
  search for a feasible vector pair in the pair of sets $W^{(\delta_i)}_{\rm end}(\mathtt{a}_i, d_i, m_i)$, $i = 1, 2$
end for.

1.8 A Complete Algorithm for the Case of Three Leaf 2-Branches

We briefly summarize how to use the procedures described thus far to obtain an algorithm. Our global constants a resource vector $\boldsymbol{x}^* = (\boldsymbol{x}^*_{\rm in}, \boldsymbol{x}^*_{\rm ex})$ with $\boldsymbol{x}^*_{\rm in}, \boldsymbol{x}^*_{\rm ex} \in \mathbb{Z}^{\Lambda\cup\Gamma\cup{\rm Bc}\cup{\rm Dg}}$ and an integer dia*.

Algorithm ThreeLeafBranchCompleteAlgorithm(Global constants: $\boldsymbol{x} = (\boldsymbol{x}^*_{\rm in}, \boldsymbol{x}^*_{\rm ex}), {\rm dia}^*$)
$\delta_3 := \sum_{\mathtt{a}\in\Lambda} \boldsymbol{x}^*_{\rm in}(\mathtt{a}) - {\rm dia}^* + 2$;
Compute the sets $W^{(0)}_{\rm end}(\mathtt{a}, d, m)$ **for each** $\mathtt{a} \in \Lambda$, $d \in [1, {\rm val}(\mathtt{a}) - 1]$, $m \in [d, {\rm val}(\mathtt{a}) - 1]$;
Compute the sets $W^{(0)}_{\rm inl}(\mathtt{a}, d, m)$ **for each** $\mathtt{a} \in \Lambda$, $d \in [0, {\rm val}(\mathtt{a}) - 2]$, $m \in [d, {\rm val}(\mathtt{a}) - 2]$;
Compute the sets $W^{(0)}_{\rm inl+3}(\mathtt{a}, d, m)$ **for each** $\mathtt{a} \in \Lambda$, $d \in [0, {\rm val}(\mathtt{a}) - 3]$, $m \in [d, {\rm val}(\mathtt{a}) - 3]$;
for each $h \in [1, {\rm dia}^* - 7 - \delta_3]$ and tuple $(\mathtt{a}_1, d_1, m_1, \mathtt{a}_2, d_2, m_2)$ with $\mathtt{a}_i \in \Lambda$, $d_i \in [1, {\rm val}(\mathtt{a}_i) - 1]$,
    $m_i \in [d_i, {\rm val}(\mathtt{a}_i) - 1], i = 1, 2$ **do**
  Compute the sets $W^{(h)}_{\rm inl}(\mathtt{a}_1, d_1, m_1, \mathtt{a}_2, d_2, m_2)$
end for;
Compute the sets $W^{(h)}_{\rm end}(\mathtt{a}, d, m)$ **for each** $\mathtt{a} \in \Lambda$, $d \in [1, {\rm val}(a) - 1]$, $m \in [d, {\rm val}(a) - 1]$
    and $h \in [1, {\rm dia}^* - 6 - \delta_3]$;
/* By the above step get the sets $W^{(\delta_i)}_{\rm end}(\mathtt{a}, d, m)$, $i = 2, 3$ for $\delta_2 \in [\delta_3, \lfloor \frac{{\rm dia}^*}{2} \rfloor - 3]$ */
Compute the set $W^{(\delta_1)}_{\rm end+2}(\mathtt{a}, d,)]$ **for each** $\mathtt{a} \in \Lambda, d \in [1, {\rm val}(\mathtt{a}) - 2]$, $m \in [d, {\rm val}(\mathtt{a}) - 2]$,
    $\delta_1 \in [\lceil \frac{{\rm dia}^*}{2} - 3 \rceil, {\rm dia}^* - 6 - \delta_3]$;
Compute the set $W^{(\delta_1+1)}_{\rm main}(\mathtt{a}, d, m)$ **for each** $\mathtt{a} \in \Lambda, d \in [2, {\rm val}(\mathtt{a}) - 1]$, $m \in [d, {\rm val}(\mathtt{a}) - 1]$,
    $\delta_1 \in [\lceil \frac{{\rm dia}^*}{2} - 3 \rceil, {\rm dia}^* - 6 - \delta_3]$;
for each two triplets $(\mathtt{a}_i, d_i, m_i)$ with $\mathtt{a}_i \in \Lambda$, $d_1 \in [2, {\rm val}(\mathtt{a}_1) - 1]$,
    $d_2 \in [1, {\rm val}(\mathtt{a}_2) - 1]$, $m_1 \in [d_1, {\rm val}(\mathtt{a}_1) - 1]$, $m_2 \in [d_2, {\rm val}(\mathtt{a}_2) - 1]$,
    $\delta_1 \in [\lceil \frac{{\rm dia}^*}{2} - 3 \rceil, {\rm dia}^* - 6 - \delta_3]$ **do**
  search for a feasible vector pair in the pair of sets $W^{(\delta_1+1)}_{\rm main}(\mathtt{a}_1, d_1, m_1)$ and $W^{(\delta_3)}_{\rm end}(\mathtt{a}_2, d_2, m_2)$
end for.