

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 $V(H) = \{v_1, v_2, \dots, v_n\}$ be such that $\deg_H(v_n) = 1$. We say that G is rooted at v_1 . Let $\text{pred} : [2, n] \rightarrow [1, n-1]$ be a bijection such that for $k \in [2, n]$, $v_k v_{\text{pred}(k)} \in E(H)$. We call the alternating sequence $(\alpha(v_1), \beta(v_{\text{pred}(2)}v_2), \alpha(v_2), \dots, \beta(v_{\text{pred}(n)}v_n), \alpha(v_n))$ the *sequence representation* of G .

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

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

Algorithm SEQMAP(\mathbf{x}^*, δ)

Input: A vector $\mathbf{x}^* = (\mathbf{x}_{\text{in}}^*, \mathbf{x}_{\text{ex}}^*)$ with $\mathbf{x}_{\text{in}}^*, \mathbf{x}_{\text{ex}}^* \in \mathbb{Z}^{\Lambda \cup \Gamma \cup \text{Bc} \cup \text{Dg}}$, an integer δ .

Output: The set $\mathcal{W}^{(\delta)}(\mathbf{x}^*)$ of vectors and a set of sequence representations

that contains all sequence representation of an acyclic graph G

with $\mathbf{f}_{\mathbf{t}}(G) = \mathbf{w}_{\mathbf{t}}^G$, $\mathbf{t} \in \{\text{in}, \text{ex}\}$, for each vector $\mathbf{w}^G \in \mathcal{W}^{(\delta)}(\mathbf{x}^*)$,

where the set of these sequences is stored in a trie.

Let $\mathbf{nb}[\mathbf{a}] := \sum_{\gamma=(\mathbf{a}, \mathbf{b}, k) \in \Gamma: \mathbf{b} \neq \mathbf{a} \in \Lambda} \mathbf{x}_{\text{ex}}^*(\gamma) + 2 \sum_{\gamma=(\mathbf{a}, \mathbf{a}, k) \in \Gamma} \mathbf{x}_{\text{ex}}^*(\gamma)$ for each element $\mathbf{a} \in \Lambda$ with $\mathbf{x}_{\text{ex}}^*(\mathbf{a}) \geq 1$;

for each $t = \mathbf{a} \in \Lambda$ **do**

$\text{Cld}_t := \text{Leaf}_t := \emptyset$;

for each tuple $\gamma \in \Gamma$ such that $\gamma = (\mathbf{a}, \mathbf{b}, k)$ for some $\mathbf{b} \in \Lambda$ and $k \in [1, 3]$ **do**

if $\mathbf{x}_{\text{ex}}^*(\mathbf{b}) \geq 1$, $\mathbf{x}_{\text{ex}}^*(\gamma) \geq 1$ and $\mathbf{x}_{\text{in}}^*(\mathbf{a}) \geq 1$ **then**

 Set $\mathbf{w}^0 = (\mathbf{w}_{\text{in}}^0, \mathbf{w}_{\text{ex}}^0)$ with $\mathbf{w}_{\text{in}}^0, \mathbf{w}_{\text{ex}}^0 \in \mathbb{Z}_+^{\Lambda \cup \Gamma \cup \text{Bc} \cup \text{Dg}}$ to be the vector such that all entries are 0;

if $\text{TRIE}(k, \mathbf{b}, \mathbf{w}_{\text{in}}^0 + \mathbf{1}_{\mathbf{a}}, \mathbf{w}_{\text{ex}}^0 + \mathbf{1}_{\mathbf{b}} + \mathbf{1}_{\gamma}, \mathbf{nb} - \mathbf{1}_{\mathbf{b}}, \delta - 1)$ returns a node v_{γ} and a leaf set Leaf_{γ} **then**

$\text{Leaf}_t := \text{Leaf}_t \cup \text{Leaf}_{\gamma}$; $\text{Cld}_t := \text{Cld}_t \cup \{v_{\gamma}\}$

endif

endif

endfor;

if $\text{Cld}_t \neq \emptyset$ **then**

Create a new node u_t as the parent of nodes in Cld_t ;
Sort the leaves $u \in \text{Leaf}_t$ in lexicographically descending order
with respect to $\text{key}(u) = (\mathbf{w}_u, \mathbf{a}_u, h_u)$;
Partition Leaf_t into subsets $\text{Leaf}_t^{(i)}$, $i = 1, 2, \dots, m_t$ so that $\text{key}(u) = \text{key}(u')$
if and only if $u, u' \in \text{Leaf}_t^{(i)}$ for some i ;
For each $i = 1, 2, \dots, m_t$, create a new node $u_{t,i}$ (called a superleaf) to the leaves in $\text{Leaf}_t^{(i)}$
and define $\text{key}(u_{t,i})$ to be $\text{key}(u) = (\mathbf{w}_u, \mathbf{a}_u, h_u)$ for a leaf $u \in \text{Leaf}_t^{(i)}$
endif;
Set $\text{W}^{(\delta)}[\mathbf{x}^*, t]$ to be the set of vectors $\mathbf{w} = \text{key}_1(u_{t,i})$ for all superleaves $u_{t,i}$
endfor;
Output $\{\text{W}^{(\delta)}[\mathbf{x}^*, t] \mid t \in \Lambda\}$ as $\mathcal{W}^{(\delta)}(\mathbf{x}^*)$.

Recursive Procedure $\text{TRIE}(h, \mathbf{a}, \mathbf{w}, \mathbf{nb}, \delta)$

Input: A vector $\mathbf{x}^* = (\mathbf{x}_{\text{in}}^*, \mathbf{x}_{\text{ex}}^*)$ with $\mathbf{x}_{\text{in}}^*, \mathbf{x}_{\text{ex}}^* \in \mathbb{Z}^{\Lambda \cup \Gamma \cup \text{Bc} \cup \text{Dg}}$ (a global constant),
an integer $h \in [1, 3]$, an element $\mathbf{a} \in \Lambda$,
a vector $\mathbf{w} = (\mathbf{w}_{\text{in}}, \mathbf{w}_{\text{ex}})$ with $\mathbf{w}_{\text{in}}, \mathbf{w}_{\text{ex}} \in \mathbb{Z}_+^{\Lambda \cup \Gamma \cup \text{Bc} \cup \text{Dg}}$,
a vector $\mathbf{nb} \in \mathbb{Z}_+^\Lambda$, and an integer $\delta \geq 0$.

Output: The set $\{\mathbf{w}^G = (\mathbf{w}_{\text{in}}^G, \mathbf{w}_{\text{ex}}^G) \in \mathcal{W}^{(\delta)}(\mathbf{x}^*) \mid \mathbf{w}_{\text{ex}}^G \geq \mathbf{w}_{\text{ex}}\}$ of vectors and a set of sequence
representations of chemical graphs that contains all graphs G on $\delta + 1$ vertices
rooted at atom \mathbf{a} , where the set of these sequences is stored in a trie.

A trie that stores all sequences of length δ from atom \mathbf{a}

with a j -bond ($j \in [1, \text{val}(\mathbf{a}) - h]$) under resource bounds of $\mathbf{x}^* - \mathbf{w}$;

if $\delta = 0$ **then**

Create a new leaf node u with $\text{key}(u) = (\mathbf{w}, \mathbf{a}, h)$, return u and a leaf set $\text{Leaf} := \{u\}$

else

$\text{Cld} := \text{Leaf} := \emptyset$;

for each tuple $\gamma = (\mathbf{a}, \mathbf{b}, k) \in \Gamma$ **do**

if $h + k \leq \text{val}(\mathbf{a})$, $\mathbf{w}_{\text{ex}}(\mathbf{b}) < \mathbf{x}_{\text{ex}}^*(\mathbf{b})$, $\mathbf{w}_{\text{ex}}(\gamma) < \mathbf{x}_{\text{ex}}^*(\gamma)$,

$\mathbf{x}_{\text{ex}}^*(\mathbf{a}) - \mathbf{w}_{\text{ex}}(\mathbf{a}) \leq \mathbf{nb}[\mathbf{a}] - 1$ **then**

if $\text{TRIE}(k + h, \mathbf{b}, \mathbf{w}_{\text{in}}, \mathbf{w}_{\text{ex}} + \mathbf{1}_{\mathbf{b}} + \mathbf{1}_{\gamma} + \mathbf{1}_{\mu}, \mathbf{nb} - \mathbf{1}_{\mathbf{a}} - \mathbf{1}_{\mathbf{b}}, \delta - 1)$ returns a node v and
a leaf set Leaf_v **then**

$\text{Cld} := \text{Cld} \cup \{v\}$; $\text{Leaf} := \text{Leaf} \cup \text{Leaf}_v$

endif

endif

endfor;

if $\text{Cld} = \emptyset$ **then**

Return **empty**

endif

endif.

1.2 Generating All Fringe Trees

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

FRINGETREEWEIGHTVECTORS(\mathbf{a})

Input: A vector $\mathbf{x}^* = (\mathbf{x}_{\text{in}}^*, \mathbf{x}_{\text{ex}}^*)$ with $\mathbf{x}_{\text{in}}^*, \mathbf{x}_{\text{ex}}^* \in \mathbb{Z}_+^{\Lambda \cup \Gamma \cup \text{Bc} \cup \text{Dg}}$ and
an element $\mathbf{a} \in \Lambda$ such that $\mathbf{x}_{\text{in}}^*[\mathbf{a}] \geq 1$;

Output: The sets $W_{\text{end}}^{(0)}(\mathbf{a}, d, m)$ (resp., $W_{\text{inl}}^{(0)}(\mathbf{a}, d, m)$ and $W_{\text{inl}+3}^{(0)}(\mathbf{a}, d, m)$)
 $d \in [1, \text{val}(\mathbf{a}) - 1]$ (resp., $d \in [0, \text{val}(\mathbf{a}) - 2]$ and $d \in [0, \text{val}(\mathbf{a}) - 3]$) and
 $m \in [d, \text{val}(\mathbf{a}) - 1]$ (resp., $m \in [d, \text{val}(\mathbf{a}) - 2]$ and $m \in [d, \text{val}(\mathbf{a}) - 3]$)
and for each vector \mathbf{w} in these sets, one sample tree $T_{\mathbf{w}}$ and the number $n_{\mathbf{w}}$ 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_{root} of v_r is 1 (i.e., v_r has exactly one child v_c),

$\mathbf{f}_{\text{ex}}(T) \leq \mathbf{x}_{\text{ex}}^*$ and $\mathbf{f}_{\text{in}}(T) = \mathbf{0} + \mathbf{1}_{\mathbf{a}}$,

the degree d_c of child v_c and the multiplicity k of edge $e_{\text{root}} = v_r v_c$

satisfy the following:

$\mathbf{f}_{\text{ex}[\text{Bc}]}(T) - \mathbf{1}_{\mu} \leq \mathbf{x}_{\text{ex}[\text{Bc}]}^*$ for the bond-configuration $\mu = (1, d_c, k)$ of edge e_{root} ;

/* Using recursive algorithm SEQMAP to enumerate these */

Let $\mathcal{T} = \{(T_i, k_i, d_i, \mathbf{w}_{\text{in}}^i, \mathbf{w}_{\text{ex}}^i) \mid i = 1, 2, \dots, q\}$ 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 , $\mathbf{w}_{\text{in}}^i = \mathbf{f}_{\text{in}}(T_i)$, and

$\mathbf{w}_{\text{ex}}^i = \mathbf{f}_{\text{ex}}(T_i) - \mathbf{1}_{\mu}$ for the bond-configuration μ of edge $e_{\text{root}} = v_r v_c$;

Step 2: Enumerate all fringe-trees T with $d_{\text{root}} \in [1, 2, 3]$ as follows:

$W[\mathbf{a}, d, m] := \emptyset$ for $d \in [1, \text{val}(\mathbf{a}) - 1]$, $m \in [d, \text{val}(\mathbf{a}) - d]$;

Let $\text{dg}^+ := 1$ (resp., $\text{dg}^+ := 2$ and $\text{dg}^+ := 3$);

/* $\text{dg}^+ := 3$ is used for the case of three leaf 2-branches */

for each $i \in [1, q]$ **do**

if $|V(T_i)| \leq 4$, $\mathbf{w}_{\text{in}}^i + \mathbf{1}_{\text{dg}^++1} \leq \mathbf{x}_{\text{in}}^*$ and $\mathbf{w}_{\text{ex}}^i + \mathbf{1}_{\mu(i)} \leq \mathbf{x}_{\text{ex}}^*$ hold for $\mu(i) := (d_i, \text{dg}^+ + 1, k_i)$ **then**

/* Also test if the height of the tree T_i is exactly equal to 2 while

constructing $W_{\text{end}}^{(0)}(\mathbf{a}, d, m)$ */

Let $\mathbf{w} := (\mathbf{w}_{\text{in}}^i + \mathbf{1}_{\text{dg}^++1}, \mathbf{w}_{\text{ex}}^i + \mathbf{1}_{\mu(i)})$;

if $\mathbf{w} \in W[\mathbf{a}, 1, k_i]$ **then** $n_{\mathbf{w}} := n_{\mathbf{w}} + 1$

else $W[\mathbf{a}, 1, k_i] := W[\mathbf{a}, 1, k_i] \cup \{\mathbf{w}\}$; $T_{\mathbf{w}} := T_i$; $n_{\mathbf{w}} := 1$ **endif**

endif;

for each $j \in [i, q]$ **do**

if $k_i + k_j \leq \text{val}(\mathbf{a}) - \text{dg}^+$ **then**

for each $h \in [j, q]$ **do**

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

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

1.3 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 $\mathbf{a} \in \Lambda$, integers $d_{\mathbf{a}} \in [1, \text{val}(\mathbf{a}) - 1]$, and $m_{\mathbf{a}} \in [d_{\mathbf{a}}, \text{val}(\mathbf{a}) - 1]$ we give a procedure to compute the set $W_{\text{end}}^{(\delta)}(\mathbf{a}, d_{\mathbf{a}}, m_{\mathbf{a}})$.

COMPUTEENDSUBTREEONE(\mathbf{a}, d, m, δ)

Input: Element $\mathbf{a} \in \Lambda$, integer $d \in [1, \text{val}(\mathbf{a}) - 1]$, $m \in [d, \text{val}(\mathbf{a}) - 1]$, $\delta \geq 1$.

/* Global data: A vector $\mathbf{x}^* = (\mathbf{x}_{\text{in}}^*, \mathbf{x}_{\text{ex}}^*)$ with $\mathbf{x}_{\text{in}}^*, \mathbf{x}_{\text{ex}}^* \in \mathbb{Z}^{\Lambda \cup \Gamma \cup \text{Bc} \cup \text{Dg}}$, the collection

$\mathcal{W}_{\text{inl}}^{(0)}$ of vector sets $W_{\text{inl}}^{(0)}(\mathbf{a}, d - 1, m_{\mathbf{a}})$, $m_{\mathbf{a}} \in [d - 1, \text{val}(\mathbf{a}) - 2]$

$\mathcal{W}_{\text{end}}^{(\delta-1)}$ of vector sets $W_{\text{end}}^{(\delta-1)}(\mathbf{a}_1, d_1, m_1)$, $\mathbf{a}_1 \in \Lambda$, $d_1 \in [1, \text{val}(\mathbf{a}_1) - 1]$, $m_1 \in [d_1, \text{val}(\mathbf{a}_1) - 1]$ and

for each vector \mathbf{w} in these sets, a sample tree $T_{\mathbf{w}}$ and the number $n_{\mathbf{w}}$ of samples trees with vector \mathbf{w} . */

Output: The set $W_{\text{end}}^{(\delta)}(\mathbf{a}, d, m)$, where we store each vector $\mathbf{w} \in W_{\text{end}}^{(\delta)}(\mathbf{a}, d, m)$, a sample tree $T_{\mathbf{w}}$ and number $n_{\mathbf{w}}$ of trees with vector \mathbf{w} in a trie.

$W := \emptyset$;

for each triplet $(\mathbf{b}, d_{\mathbf{b}}, m_{\mathbf{b}})$ **do**

for each triplet $(\mathbf{a}, d - 1, m_{\mathbf{a}})$ **do**

for each $\mathbf{w}^{\mathbf{b}} = (\mathbf{w}_{\text{in}}^{\mathbf{b}}, \mathbf{w}_{\text{ex}}^{\mathbf{b}}) \in W_{\text{end}}^{(\delta-1)}(\mathbf{b}, d_{\mathbf{b}}, m_{\mathbf{b}})$, **do**

for each $m' \in [1, 3]$ such that

- $\gamma = (\mathbf{a}, \mathbf{b}, m') \in \Gamma$,

- $\mu = (d + 1, d_{\mathbf{b}} + 1, m') \in \text{Bc}$ and

- $m_{\mathbf{a}} + m' = m$, $m_{\mathbf{a}} + m' + 1 \leq \text{val}(\mathbf{a})$ and $m' + m_{\mathbf{b}} \leq \text{val}(\mathbf{b})$ **do**

for each $\mathbf{w}^{\mathbf{a}} = (\mathbf{w}_{\text{in}}^{\mathbf{a}}, \mathbf{w}_{\text{ex}}^{\mathbf{a}}) \in W_{\text{inl}}^{(0)}(\mathbf{a}, d - 1, m_{\mathbf{a}})$ **do**

$\mathbf{w}_{\text{in}} := \mathbf{w}_{\text{in}}^{\mathbf{a}} + \mathbf{w}_{\text{in}}^{\mathbf{b}} + \mathbf{1}_{\mu} + \mathbf{1}_{\gamma}$;

$\mathbf{w}_{\text{ex}} := \mathbf{w}_{\text{ex}}^{\mathbf{a}} + \mathbf{w}_{\text{ex}}^{\mathbf{b}}$;

if $\mathbf{w} = (\mathbf{w}_{\text{in}}, \mathbf{w}_{\text{ex}}) \in W$ **then** $n_{\mathbf{w}} = n_{\mathbf{w}} + n_{\mathbf{w}^{\mathbf{a}}} \cdot n_{\mathbf{w}^{\mathbf{b}}}$

else

Let T be the tree obtained by joining the roots of $T_{\mathbf{w}^{\mathbf{a}}}$ and $T_{\mathbf{w}^{\mathbf{b}}}$
by an edge of multiplicity m ;

$W := W \cup \{(\mathbf{w}_{\text{in}}, \mathbf{w}_{\text{ex}})\}$; $T_{\mathbf{w}} := T$; $n_{\mathbf{w}} := n_{\mathbf{w}^{\mathbf{a}}} \cdot n_{\mathbf{w}^{\mathbf{b}}}$

end if

end for

end for

end for

end for

end for;

Output W as $W_{\text{end}}^{(\delta)}(\mathbf{a}, d, m)$, and for each $\mathbf{w} \in W$, $T_{\mathbf{w}}$ and $n_{\mathbf{w}}$.

Computing vectors of end-subtrees with two fictitious edge

For an integer $\delta \geq 2$, element $\mathbf{a} \in \Lambda$, integers $d_{\mathbf{a}} \in [1, \text{val}(\mathbf{a}) - 2]$, and $m_{\mathbf{a}} \in [d_{\mathbf{a}}, \text{val}(\mathbf{a}) - 1]$ we give a procedure to compute the set $W_{\text{end}+2}^{(\delta)}(\mathbf{a}, d_{\mathbf{a}}, m_{\mathbf{a}})$.

COMPUTEENDSUBTREETWO(\mathbf{a}, d, m, δ)

Input: Element $\mathbf{a} \in \Lambda$, integer $d \in [1, \text{val}(\mathbf{a}) - 2]$, $m \in [d, \text{val}(\mathbf{a}) - 1]$, $\delta \geq 2$.

/* Global data: A vector $\mathbf{x}^* = (\mathbf{x}_{\text{in}}^*, \mathbf{x}_{\text{ex}}^*)$ with $\mathbf{x}_{\text{in}}^*, \mathbf{x}_{\text{ex}}^* \in \mathbb{Z}^{\Lambda \cup \Gamma \cup \text{Bc} \cup \text{Dg}}$, the collection

$\mathcal{W}_{\text{inl}+3}^{(0)}$ of vector sets $W_{\text{inl}+3}^{(0)}(\mathbf{a}, d - 1, m_{\mathbf{a}})$, $m_{\mathbf{a}} \in [d - 1, \text{val}(\mathbf{a}) - 3]$

$\mathcal{W}_{\text{end}}^{(\delta-1)}$ of vector sets $W_{\text{end}}^{(\delta-1)}(\mathbf{a}_1, d_1, m_1)$, $\mathbf{a}_1 \in \Lambda$, $d_1 \in [1, \text{val}(\mathbf{a}_1) - 1]$, $m_1 \in [d_1, \text{val}(\mathbf{a}_1) - 1]$ and for each vector w in these sets, a sample tree $T_{\mathbf{w}}$ and the number $n_{\mathbf{w}}$ of samples trees with vector \mathbf{w} . */

Output: The set $W_{\text{end}+2}^{(\delta)}(\mathbf{a}, d, m)$, where we store each vector $\mathbf{w} \in W_{\text{end}+2}^{(\delta)}(\mathbf{a}, d, m)$, a sample tree $T_{\mathbf{w}}$ and number $n_{\mathbf{w}}$ of trees with vector \mathbf{w} in a trie.

$W := \emptyset$;

for each triplet $(\mathbf{b}, d_{\mathbf{b}}, m_{\mathbf{b}})$ **do**

for each triplet $(\mathbf{a}, d - 1, m_{\mathbf{a}})$ **do**

for each $\mathbf{w}^{\mathbf{b}} = (\mathbf{w}_{\text{in}}^{\mathbf{b}}, \mathbf{w}_{\text{ex}}^{\mathbf{b}}) \in W_{\text{end}}^{(\delta-1)}(\mathbf{b}, d_{\mathbf{b}}, m_{\mathbf{b}})$, **do**

for each $m' \in [1, 3]$ such that

- $\gamma = (\mathbf{a}, \mathbf{b}, m') \in \Gamma$,

- $\mu = (d + 2, d_{\mathbf{b}} + 1, m') \in \text{Bc}$ and

- $m_{\mathbf{a}} + m' = m$, $m_{\mathbf{a}} + m' + 2 \leq \text{val}(\mathbf{a})$ and $m' + m_{\mathbf{b}} \leq \text{val}(\mathbf{b})$ **do**

for each $\mathbf{w}^{\mathbf{a}} = (\mathbf{w}_{\text{in}}^{\mathbf{a}}, \mathbf{w}_{\text{ex}}^{\mathbf{a}}) \in W_{\text{inl}+3}^{(0)}(\mathbf{a}, d - 1, m_{\mathbf{a}})$ **do**

$\mathbf{w}_{\text{in}} := \mathbf{w}_{\text{in}}^{\mathbf{a}} + \mathbf{w}_{\text{in}}^{\mathbf{b}} + \mathbf{1}_{\mu} + \mathbf{1}_{\gamma}$;

$\mathbf{w}_{\text{ex}} := \mathbf{w}_{\text{ex}}^{\mathbf{a}} + \mathbf{w}_{\text{ex}}^{\mathbf{b}}$;

if $\mathbf{w} = (\mathbf{w}_{\text{in}}, \mathbf{w}_{\text{ex}}) \in W$ **then** $n_{\mathbf{w}} = n_{\mathbf{w}} + n_{\mathbf{w}^{\mathbf{a}}} \cdot n_{\mathbf{w}^{\mathbf{b}}}$

else

Let T be the tree obtained by joining the roots of $T_{\mathbf{w}^{\mathbf{a}}}$ and $T_{\mathbf{w}^{\mathbf{b}}}$

by an edge of multiplicity m ;

$W := W \cup \{(\mathbf{w}_{\text{in}}, \mathbf{w}_{\text{ex}})\}$; $T_{\mathbf{w}} := T$; $n_{\mathbf{w}} := n_{\mathbf{w}^{\mathbf{a}}} \cdot n_{\mathbf{w}^{\mathbf{b}}}$

end if

end for

end for

end for

end for

end for;

Output W as $W_{\text{end}+2}^{(\delta)}(\mathbf{a}, d, m)$, and for each $\mathbf{w} \in W$, $T_{\mathbf{w}}$ and $n_{\mathbf{w}}$.

1.4 Computing Weight Vectors of Main-Subtrees

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

COMPUTEMAINTREE(\mathbf{a}, d, m, δ)

Input: Element $\mathbf{a} \in \Lambda$, integer $d \in [2, \text{val}(\mathbf{a}) - 1]$, $m \in [d, \text{val}(\mathbf{a}) - 1]$, $\delta \geq 1$.

/* Global data: An integer dia^* , a vector $\mathbf{x}^* = (\mathbf{x}_{\text{in}}^*, \mathbf{x}_{\text{ex}}^*)$ with $\mathbf{x}_{\text{in}}^*, \mathbf{x}_{\text{ex}}^* \in \mathbb{Z}^{\Lambda \cup \Gamma \cup \text{Bc} \cup \text{Dg}}$,
the collection $\mathcal{W}_{\text{end}+2}^{(\delta+1)}$ of vector sets $W_{\text{end}+2}^{(\delta+1)}(\mathbf{a}, d-1, m_{\mathbf{a}})$, $m_{\mathbf{a}} \in [d-1, \text{val}(\mathbf{a}) - 2]$
 $\mathcal{W}_{\text{end}}^{(\delta')}$ of vector sets $W_{\text{end}}^{(\delta')}(\mathbf{a}_1, d_1, m_1)$, $\mathbf{a}_1 \in \Lambda$, $d_1 \in [1, \text{val}(\mathbf{a}_1) - 1]$, $m_1 \in [d_1, \text{val}(\mathbf{a}_1) - 1]$
such that $\delta + \delta' + 2 = \text{dia}^* - 4$ and
for each vector \mathbf{w} in these sets, a sample tree $T_{\mathbf{w}}$ and the number $n_{\mathbf{w}}$ of samples trees
with vector \mathbf{w} . */

Output: The set $W_{\text{main}}^{(\delta+1)}(\mathbf{a}, d, m)$, where we store each vector $\mathbf{w} \in W_{\text{main}}^{(\delta+1)}(\mathbf{a}, d, m)$, a sample tree $T_{\mathbf{w}}$ and number $n_{\mathbf{w}}$ of trees with vector \mathbf{w} in a trie.

$W := \emptyset$;

for each triplet $(\mathbf{b}, d_{\mathbf{b}}, m_{\mathbf{b}})$ **do**

for each triplet $(\mathbf{a}, d-1, m_{\mathbf{a}})$ **do**

for each $\mathbf{w}^{\mathbf{b}} = (\mathbf{w}_{\text{in}}^{\mathbf{b}}, \mathbf{w}_{\text{ex}}^{\mathbf{b}}) \in W_{\text{end}}^{(\delta')}(\mathbf{b}, d_{\mathbf{b}}, m_{\mathbf{b}})$, **do**

for each $m' \in [1, 2]$ such that

 - $\gamma = (\mathbf{a}, \mathbf{b}, m') \in \Gamma$,

 - $\mu = (d+1, d_{\mathbf{b}}+1, m') \in \text{Bc}$ and

 - $m_{\mathbf{a}} + m' = m, m_{\mathbf{a}} + m' + 1 \leq \text{val}(\mathbf{a})$ and $m' + m_{\mathbf{b}} \leq \text{val}(\mathbf{b})$ **do**

for each $\mathbf{w}^{\mathbf{a}} = (\mathbf{w}_{\text{in}}^{\mathbf{a}}, \mathbf{w}_{\text{ex}}^{\mathbf{a}}) \in W_{\text{end}+2}^{(\delta+1)}(\mathbf{a}, d-1, m_{\mathbf{a}})$ **do**

$\mathbf{w}_{\text{in}} := \mathbf{w}_{\text{in}}^{\mathbf{a}} + \mathbf{w}_{\text{in}}^{\mathbf{b}} + \mathbf{1}_{\mu} + \mathbf{1}_{\gamma}$;

$\mathbf{w}_{\text{ex}} := \mathbf{w}_{\text{ex}}^{\mathbf{a}} + \mathbf{w}_{\text{ex}}^{\mathbf{b}}$;

if $\mathbf{w} = (\mathbf{w}_{\text{in}}, \mathbf{w}_{\text{ex}}) \in W$ **then** $n_{\mathbf{w}} = n_{\mathbf{w}} + n_{\mathbf{w}^{\mathbf{a}}} \cdot n_{\mathbf{w}^{\mathbf{b}}}$

else

 Let T be the tree obtained by joining the roots of $T_{\mathbf{w}^{\mathbf{a}}}$ and $T_{\mathbf{w}^{\mathbf{b}}}$

 by an edge of multiplicity m ;

$W := W \cup \{(\mathbf{w}_{\text{in}}, \mathbf{w}_{\text{ex}})\}$; $T_{\mathbf{w}} := T$; $n_{\mathbf{w}} := n_{\mathbf{w}^{\mathbf{a}}} \cdot n_{\mathbf{w}^{\mathbf{b}}}$

end if

end for

end for

end for

end for

end for;

Output W as $W_{\text{main}}^{(\delta+1)}(\mathbf{a}, d, m)$, and for each $\mathbf{w} \in W$, $T_{\mathbf{w}}$ and $n_{\mathbf{w}}$.

1.5 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 $\delta_1 = \lfloor \frac{\text{dia}^* - 5}{2} \rfloor$ and $\delta_2 = \text{dia}^* - 5 - \delta_1 = \lceil \frac{\text{dia}^* - 5}{2} \rceil$. and compute feasible pair of vectors $\mathbf{w}^i = (\mathbf{w}_{\text{in}}^i, \mathbf{w}_{\text{ex}}^i) \in W_{\text{end}}^{(\delta_i)}(\mathbf{a}_i, d_i, m_i)$, $\mathbf{a}_i \in \Lambda$, $d_i \in [1, \text{val}(\mathbf{a}_i) - 1]$, $m_i \in [d_i, \text{val}(\mathbf{a}_i) - 1]$, $i = 1, 2$.

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

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

Algorithm COMBINE(global data: $\mathbf{x}^* = (\mathbf{x}_{\text{in}}^*, \mathbf{x}_{\text{ex}}^*)$)

Input: Two sets W_1 and W_2 such that $W_1(\mathbf{a}_1, d_1, m_1) = W_{\text{end}}^{(\delta_1)}(\mathbf{a}_1, d_1, m_1)$ and

$W_2(\mathbf{a}_2, d_2, m_2) = W_{\text{end}}^{(\delta_2)}(\mathbf{a}_2, d_2, m_2)$ (resp., $W_1(\mathbf{a}_1, d_1, m_1) = W_{\text{main}}^{(\delta_1+1)}(\mathbf{a}_1, d_1, m_1)$ and

$W_2(\mathbf{a}_2, d_2, m_2) = W_{\text{end}}^{(\delta_3)}(\mathbf{a}_2, d_2, m_2)$)

for the case of two leaf 2-branches (resp., three leaf 2-branches), where we assume that all

vectors $\mathbf{z} = (\mathbf{z}_{\text{in}}, \mathbf{z}_{\text{ex}})$ with $\mathbf{z}_{\text{in}}, \mathbf{z}_{\text{ex}} \in \mathbb{Z}^{\Lambda \cup \Gamma \cup \text{Bc} \cup \text{Dg}}$ in each set $W_i(\mathbf{a}_i, d_i, m_i)$, $i = 1, 2$

have been sorted in a lexicographical order.

Output: All feasible pairs $(\mathbf{z}_1, \mathbf{z}_2)$ 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 $\gamma = (\mathbf{a}_1, \mathbf{a}_2, k) \in \Gamma$ and $\mu = (d_1 + 1, d_2 + 1, k) \in \text{Bc}$ with

$m_i + k \leq \text{val}(\mathbf{a}_i)$, $i = 1, 2$ **do**

Let L_1 denote the sorted list of vectors in $W_1(\mathbf{a}_1, d_1, m_1)$;

Construct the set $\bar{W} := \{\bar{\mathbf{z}} \mid \mathbf{z} \in W_2(\mathbf{a}_2, d_2, m_2)\}$ of the (γ, μ) -complement vectors;

Sort the vectors in \bar{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 $\mathbf{z}^1, \mathbf{z}^2$ of vectors with $\mathbf{z}^1 = \mathbf{z}^2$

Output $(\mathbf{z}^1, \mathbf{z}^2)$ as a feasible pair;

Let T be a tree obtained by joining the roots of $T_{\mathbf{z}^1}$ and $T_{\bar{\mathbf{z}}^2}$ with bond configuration γ ;

/* Execute the next for the case of two leaf 2-branches */

$\ell := \ell + \lceil (n_{\mathbf{z}^1} \cdot n_{\bar{\mathbf{z}}^2}) / 2 \rceil$

/* Execute the next for the case of three leaf 2-branches */

$\ell := \ell + \lceil (n_{\mathbf{z}^1} \cdot n_{\bar{\mathbf{z}}^2}) / 6 \rceil$

endfor;

Output ℓ .

1.6 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 $\mathbf{x}^* = (\mathbf{x}_{\text{in}}^*, \mathbf{x}_{\text{ex}}^*)$ with $\mathbf{x}_{\text{in}}^*, \mathbf{x}_{\text{ex}}^* \in \mathbb{Z}^{\Lambda \cup \Gamma \cup \text{Bc} \cup \text{Dg}}$ and an integer dia^* .

TWOLEAFBRANCHCOMPLETEALGORITHM(Global constants: $\mathbf{x}^* = (\mathbf{x}_{\text{in}}^*, \mathbf{x}_{\text{ex}}^*)$, dia^*)

$\delta_1 := \lfloor (\text{dia}^* - 5)/2 \rfloor$, $\delta_2 := \lceil (\text{dia}^* - 5)/2 \rceil$;

Compute the sets $W_{\text{end}}^{(0)}(\mathbf{a}, d, m)$ **for each** $\mathbf{a} \in \Lambda$, $d \in [1, \text{val}(\mathbf{a}) - 1]$, $m \in [d, \text{val}(\mathbf{a}) - 1]$;

Compute the sets $W_{\text{inl}}^{(0)}(\mathbf{a}, d, m)$ **for each** $\mathbf{a} \in \Lambda$, $d \in [0, \text{val}(\mathbf{a}) - 2]$, $m \in [d, \text{val}(\mathbf{a}) - 2]$;

Compute the sets $W_{\text{end}}^{(h)}(\mathbf{a}, d, m)$ **for each** $\mathbf{a} \in \Lambda$, $d \in [1, \text{val}(\mathbf{a}) - 1]$, $m \in [d, \text{val}(\mathbf{a}) - 1]$, $h = \delta_1, \delta_2$;

for each two triplets (\mathbf{a}_i, d_i, m_i) with $\mathbf{a}_i \in \Lambda$, $d_i \in [1, \text{val}(\mathbf{a}_i) - 1]$, $m_i \in [d_i, \text{val}(\mathbf{a}_i) - 1]$ **do**

search for a feasible vector pair in the pair of sets $W_{\text{end}}^{(\delta_i)}(\mathbf{a}_i, d_i, m_i)$, $i = 1, 2$

end for.

1.7 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 $\mathbf{x}^* = (\mathbf{x}_{\text{in}}^*, \mathbf{x}_{\text{ex}}^*)$ with $\mathbf{x}_{\text{in}}^*, \mathbf{x}_{\text{ex}}^* \in \mathbb{Z}^{\Lambda \cup \Gamma \cup \text{Bc} \cup \text{Dg}}$ and an integer dia^* .

Algorithm THREELEAFBRANCHCOMPLETEALGORITHM(Global constants: $\mathbf{x} = (\mathbf{x}_{\text{in}}^*, \mathbf{x}_{\text{ex}}^*)$, dia^*)

$\delta_3 := \sum_{\mathbf{a} \in \Lambda} \mathbf{x}_{\text{in}}^*(\mathbf{a}) - \text{dia}^* + 2$;

Compute the sets $W_{\text{end}}^{(0)}(\mathbf{a}, d, m)$ **for each** $\mathbf{a} \in \Lambda$, $d \in [1, \text{val}(\mathbf{a}) - 1]$, $m \in [d, \text{val}(\mathbf{a}) - 1]$;

Compute the sets $W_{\text{inl}}^{(0)}(\mathbf{a}, d, m)$ **for each** $\mathbf{a} \in \Lambda$, $d \in [0, \text{val}(\mathbf{a}) - 2]$, $m \in [d, \text{val}(\mathbf{a}) - 2]$;

Compute the sets $W_{\text{inl}+3}^{(0)}(\mathbf{a}, d, m)$ **for each** $\mathbf{a} \in \Lambda$, $d \in [0, \text{val}(\mathbf{a}) - 3]$, $m \in [d, \text{val}(\mathbf{a}) - 3]$;

Compute the sets $W_{\text{end}}^{(h)}(\mathbf{a}, d, m)$ **for each** $\mathbf{a} \in \Lambda$, $d \in [1, \text{val}(\mathbf{a}) - 1]$, $m \in [d, \text{val}(\mathbf{a}) - 1]$

and $h \in [1, \text{dia}^* - 6 - \delta_3]$;

/ By the above step get the sets $W_{\text{end}}^{(\delta_i)}(\mathbf{a}, d, m)$, $i = 2, 3$ for $\delta_2 \in [\delta_3, \lfloor \frac{\text{dia}^*}{2} \rfloor - 3]$ */*

Compute the set $W_{\text{end}+2}^{(\delta_1)}(\mathbf{a}, d, m)$ **for each** $\mathbf{a} \in \Lambda$, $d \in [1, \text{val}(\mathbf{a}) - 2]$, $m \in [d, \text{val}(\mathbf{a}) - 2]$,

$\delta_1 \in [\lceil \frac{\text{dia}^*}{2} \rceil - 3, \text{dia}^* - 6 - \delta_3]$;

Compute the set $W_{\text{main}}^{(\delta_1+1)}(\mathbf{a}, d, m)$ **for each** $\mathbf{a} \in \Lambda$, $d \in [2, \text{val}(\mathbf{a}) - 1]$, $m \in [d, \text{val}(\mathbf{a}) - 1]$,

$\delta_1 \in [\lceil \frac{\text{dia}^*}{2} \rceil - 3, \text{dia}^* - 6 - \delta_3]$;

for each two triplets (\mathbf{a}_i, d_i, m_i) with $\mathbf{a}_i \in \Lambda$, $d_i \in [2, \text{val}(\mathbf{a}_i) - 1]$,

$d_2 \in [1, \text{val}(\mathbf{a}_2) - 1]$, $m_1 \in [d_1, \text{val}(\mathbf{a}_1) - 1]$, $m_2 \in [d_2, \text{val}(\mathbf{a}_2) - 1]$,

$\delta_1 \in [\lceil \frac{\text{dia}^*}{2} \rceil - 3, \text{dia}^* - 6 - \delta_3]$ **do**

search for a feasible vector pair in the pair of sets $W_{\text{main}}^{(\delta_1+1)}(\mathbf{a}_1, d_1, m_1)$ and $W_{\text{end}}^{(\delta_3)}(\mathbf{a}_2, d_2, m_2)$

end for.