

Idea: in each iteration set taxonomic ID of an accession to its direct ancestor ID. If this ID is existent, the accession list associated with taxID will be merged with the one of its ancestor, else the taxID is replaced by its ancestor in the next iteration.

Algorithm 1 Sequential distribution of accessions into N equally filled bins.

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1: procedure TAXONOMICBINNING( $\text{accList}$ ,  $\text{acc2tax}$ ,  $\pi$ ,  $B$ )
2:    $\text{bins} \leftarrow \emptyset$   $\triangleright$  Dictionary with keys representing clades and values accessions
3:    $H \leftarrow 4 \cdot \lceil \frac{|\text{accList}|}{B} \rceil$   $\triangleright$  Size threshold of a bin
4:   for  $\text{acc}$  in  $\text{accList}$  do  $\triangleright$  Initial compression ensuring uniqueness of keys
5:      $\text{tax}_{\text{acc}} \leftarrow \text{acc2tax}[\text{acc}]$ 
6:     if  $\text{tax}_{\text{acc}} \notin \text{bins.keys()}$  then
7:        $\text{bins}[\text{tax}_{\text{acc}}] \leftarrow (1, [\text{acc}])$ 
8:     else
9:        $\text{bins}[\text{tax}_{\text{acc}}] \leftarrow \text{bins}[\text{tax}_{\text{acc}}] + [(1, \text{acc})]$ 
10:  while  $|\text{bins}| > B$  do  $\triangleright$  Number of clades still larger than target
11:     $\text{keys} \leftarrow \text{bins.keys().sort()}$   $\triangleright$  Handle lower-level keys first
12:     $\text{climbers} \leftarrow \emptyset$   $\triangleright$  Key-value pairs to be merged with their parent
13:     $\text{blockedSet} \leftarrow \emptyset$   $\triangleright$  Set of nodes that are parent of another key
14:    for  $\text{key} \in \text{keys}$  do
15:      if  $\text{key} \in \text{blockedSet}$  then  $\triangleright$  Node has descendants to be merged into
16:        continue
17:      if  $\pi[\text{key}] \in \text{keys}$  then  $\triangleright$  Prevent parent from being replaced
18:         $\text{blockedSet} \leftarrow \pi[\text{key}]$ 
19:         $\text{climbers} \leftarrow (\pi[\text{key}], \text{key})$ 
20:      for  $\text{parent\_key}, \text{key} \in \text{climbers}$  do
21:        if  $\text{key} \in \text{blockedList}$  then
22:          continue
23:         $\text{tax2accs}[\text{parent\_key}] \leftarrow [\text{tax2accs.pop}(\text{key})]$ 
return  $\text{tax2accs}$ 

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