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**Algorithm 2** One iteration of the Weisfeiler-Lehman subtree kernel computation on  $N$  graphs

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1: Multiset-label determination

- Assign a multiset-label  $M_i(v)$  to each node  $v$  in  $G$  which consists of the multiset  $\{l_{i-1}(u) | u \in \mathcal{N}(v)\}$ .

2: Sorting each multiset

- Sort elements in  $M_i(v)$  in ascending order and concatenate them into a string  $s_i(v)$ .
- Add  $l_{i-1}(v)$  as a prefix to  $s_i(v)$ .

3: Label compression

- Map each string  $s_i(v)$  to a compressed label using a hash function  $f : \Sigma^* \rightarrow \Sigma$  such that  $f(s_i(v)) = f(s_i(w))$  if and only if  $s_i(v) = s_i(w)$ .

4: Relabeling

- Set  $l_i(v) := f(s_i(v))$  for all nodes in  $G$ .
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