

## Simple $k$ -RF Metrics for Labeled DAGs

- “sK-RFmeasures.py” contains the code to compute pairwise  $s$ - $k$ -RF or  $m$ - $k$ -RF distances of a set of (multi-labeled) labeled DAGs stored in an input JSON file. The command line to run the code is “python3 sK-RFmeasures.py inputfile k m n”. The “inputfile” refers to a JSON file that consists of the DAGs whose pairwise distances must be computed. The parameter  $k$  is an integer that is greater than or equal to zero. The parameter  $m$  is a binary integer, where we set  $m = 0$  if we want to compute  $s$ - $k$ -RF distances and we set  $m = 1$  if we want to compute  $m$ - $k$ -RF distances. The parameter  $n$  is also a binary integer, where we set  $n = 0$  if we want to compute unnormalized distances and we set  $n = 1$  if we want to compute normalized distances.

A multi-labeled DAG  $G$  in the input file needs to be represented as  $[A, B]$ , where  $A$  is the list of nodes in  $G$  with their labels, and  $B$  is the list of edges of  $G$ . Each node  $v \in V(G)$  is represented as  $[v, a_1, \dots, a_n]$  if  $\ell(v) = \{a_1, \dots, a_n\}$ . Note that  $v$  must be in the first position of the array. Additionally, each edge from  $v \in V(G)$  to  $u \in V(G)$  is represented as  $[v, u]$ .

- “sKfunctions.py” contains the necessary functions required to run the code in “sK-RFmeasures.py”.
- “255DAGs.json” is a sample input file containing all 255 DAGs used for our clustering experiment on labeled DAGs, as described in the paper.
- “250DAGsPC\_sim.json” is a sample input file containing all 250 DAGs with the same number of edges, used for the correlation analysis of the  $s$ - $k$ -RF measures with the  $m$ - $k$ -RF measures, the generalized Kendall-tau (GKT) distance and the Katz dissimilarity, as described in the paper.
- “250DAGsPC\_dif.json” is a sample input file containing all 250 DAGs with different number of edges, used for the correlation analysis of the  $s$ - $k$ -RF measures with the  $m$ - $k$ -RF measures, the generalized Kendall-tau (GKT) distance and the Katz dissimilarity, as described in the paper.
- “240mutation\_trees.json” is a sample input file containing all 240 multi-labeled trees used for comparing clustering performances of the  $k$ -RF measures and the simple  $k$ -RF measures.

- “DAGs\_resol.json” is a sample input file containing all DAGs used to compare the  $s$ - $k$ -RF distances with the  $m$ - $k$ -RF distances to show how the latter refine the former.
- “Resol\_one\_label\_trees.json” is a sample input file containing all trees used to compare the  $s$ - $k$ -RF distances with the  $k$ -RF distances to show how the former can improve the resolution of the latter for trees with different label sets.
- “combinedtree-PC.json” is a sample input file containing all 950 trees used for the correlation analysis performed to compare the  $s$ - $k$ -RF measures with  $k$ -RF distances,  $\text{DISC}\cap$ ,  $\text{Caset}\cap$ , and GRF distances.