

Algorithm: RWR_Cluster

Data: $ListofQuerySets \leftarrow \{Lists\ of\ sets\ of\ start\ Nodes\}$
 $G \leftarrow Global\ PairWise\ BLAST\ BitScore\ Graph$

RWR Parameters:

$restart_prob = probability\ of\ returning\ to\ the\ start\ nodes$
 $threshold = repeat\ loop\ till\ L1\ error \leq threshold$
 $iter_cutoff = maximum\ number\ of\ iterations$
 $K = Step\ size$

Permutation Statistics parameters:

$num_replicates = number\ of\ replications$

Result: $ClusterMap :$

$Map(Query_Name \rightarrow Map(Node \rightarrow Scores(Statistics)))$

begin

$Cluster_Map \leftarrow Map(Query_Name \rightarrow Map(Node \rightarrow Scores))$

Random Walk Section:

forall the $QuerySet \in ListofQuerySets$

do

| $Cluster_Map \leftarrow RWR\ in\ threads(QuerySet, RWR_Parameters)$

end

Permutation Statistics Section:

$Population \leftarrow Map(Query_Name \rightarrow$

$Random_Permutation(ListofQuerySets, RWRParameters, num_replicates)$

Summarize Statistics Section:

forall the $QuerySet \in Keys(Cluster_Map)$

do

| $Cluster : Map(Node \rightarrow Scores) \leftarrow Cluster_Map(QuerySet)$

| **forall the** $c.member : members\ of\ ClusterofQuerySet$

| **do**

| | $p.value \leftarrow \frac{|scores\ from\ Population(QuerySet) \geq Score|}{size\ of\ Population}$

| | $max.norm.score \leftarrow Score\ normalized\ by\ max\ score\ in\ Cluster$

| | $species.norm.score \leftarrow$

| | $Score\ normalized\ by\ max\ score\ within\ same\ species\ in\ Cluster$

| | Update scores of $Cluster$ with [score,p.value,norm.score,species.norm.score]

| **end**

| Update $Cluster_Map$ with $Cluster$

end

end

Algorithm: *RWR_in_threads*

Data: *Queries* $\rightarrow \{\text{Set of start Nodes}\}$

Global variables:

$G \leftarrow \text{Global PairWise BLAST BitScore Graph}$

$\text{threshold} = \text{repeat loop till L1 error} \leq \text{threshold}$

$\text{iter_cutoff} = \text{repeat loop at least iteration threshold times } K = \text{Step size}$

Result: $\text{PostProbMap} = \text{Map}(s \rightarrow \text{probability to end walk at } s),$
 $s \in \text{Nodes in } G \text{ with non-zero post-probabilities}$

begin

$\text{LocalGraph} \leftarrow K - \text{Step Neighborhood of Queries in } G$

$W = \text{Adjacency matrix from LocalGraph}$

$\text{index_name_map} = \text{Map}(\text{index of } W \rightarrow \text{Query_Name})$

$\text{name_index_map} = \text{Map}(\text{Query_Name} \rightarrow \text{index of } W)$

$N = \text{Number of Start Nodes}$

$Q\text{Indices} \rightarrow \{\text{Set of indices of Queries in } W\}$

$p^0 \leftarrow \{p_i^0\} \text{ for } i \in \text{indices of } W$

$$p_i^0 = \begin{cases} \frac{1}{N}, & \text{if } i \in Q\text{Indices} \\ 0, & \text{otherwise} \end{cases}$$

$\text{normalize } W$

while $|p^{t+1} - p^t| \leq \text{threshold}$ **and** $\text{iter} \leq \text{iter_cutoff}$ **do**

$p^{t+1} = (1 - r)Wp^t + rp^0$

end

$p^{\text{final}} = p^{t+1}$

 Create a post probability map from p^{final} :

$\text{PostProbMap} = \text{Map}(s \rightarrow \text{probability to end walk at } s),$

$s \in \text{Nodes in LocalGraph with nonzero values in } p^{t+1}$

 Update Concurrent HashMap holding Results

end

Algorithm: Permutation_Statistics

Data: *ListofQuerySets* $\rightarrow \{\text{Lists of query sets}\}$
Degree_Node Map ($d \rightarrow \{\text{Set of Nodes with degree } d\}$)
Global variables:
 $G \leftarrow \text{Pairwise sequence similarity network}$

Result: *Population_Map* :
Map(Query_Name $\rightarrow \{\text{population of post probability values}\})$

Get Sample Populations for the QuerySets:

SampleSpace $\leftarrow \text{Get_SampleSpace_for_QuerySets}$ *Sets*(*ListofQuerySets*)

Permutation Statistics Section:

Population_Map $\leftarrow \text{Post rwr probability values from permuted queries}$

forall the *queryset* \in *ListofQuerySets*

do

$q.size \leftarrow \text{number of nodes in queryset}$ $q.name \leftarrow \text{name of queryset}$ **repeat**
 $\text{Perm_Query} \leftarrow \text{Randomly sample } q.size \text{ nodes from SampleSpace}[q.name]$
 $\text{Update Population_n} \leftarrow \text{RWR in threads}(\text{Perm_Query}, \text{RWR_Parameters})$
 $rep++$

until $rep \leq num_replicates$;

$\text{Update : Population_Map}[n] \leftarrow \text{Population_n}$

end

Algorithm: *Get_SampleSpace_for_QuerySets*

Data: *ListofQuerySets* $\rightarrow \{\text{Lists of QuerySets}\}$
Degree_Map ($d \rightarrow \{\text{Set of Nodes with degree } d \text{ for } G\}$)

Result: *SampleSpace_Map* : *Map(querysetid \rightarrow Set of Nodes)*

forall the *queryset* \in *ListofQuerySets*

do

queryset.size \leftarrow number of nodes in *queryset*

max.degree \leftarrow *max*(*degree*(nodes in *queryset*))

min.degree \leftarrow *min*(*degree*(nodes in *queryset*))

SampeSpace $\leftarrow \{\text{Pooled sets of nodes from Degree_Map}[\text{max.degree} + \text{range}] \text{ to Degree_Map}[\text{min.degree} - \text{range}]\}$

 Add (*querysetid* \rightarrow *SampleSpace*) map to *SampleSpace_Map*

end