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A New Approach for Clustering of Gene Sequences

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ABSTRACT

In modern days, with the development of biotechnology results in the vast amount of raw biological data. Thousands of sequence data appear every day. So to identify the similar sequence into a group is necessary for different bioinformatics problems like phylogeny construction, genomic sequence analysis, gene finding, gene mapping. Due to the massive amount of sequences, computational complexity for clustering sequences increases day by day. Here a new approach is proposed for clustering gene sequences.

CLUSTERING

Clustering is the process of identifying similar characteristics and grouping data with similar characteristics together. These groups are called clusters. Clustering approach can be viewed as extrinsic or intrinsic. Extrinsic technique implies traditional classification supervised learning algorithm in which a particular input training is used. Intrinsic algorithms do not use any a priori category labels but depend only on a similarity measure. The proposed algorithm falls into the intrinsic class. For each cluster, representative genes are identified by approximated weighted length technique. It is called CURE (Clustering Using REpresentatives) approach

PROPOSED ALGORITHM: RaTa (Definition)

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n_i = frequency of i type element in input database.
    i {A,C,T,G}
N = total occurrence of each type of element = \sum n_i
w_i = weight of i type element of gene sequence = n/N
W_q = weight of the gene sequence g = \sum w_i
I_a = lenght of the gene sequence g
W_{cmax} = weight of the highest length gene of cluster c
L_{cmax} = max(I_q) for each gene g in cluster c
ref_c = reference gene of cluster c
S(g, ref_c) = function denoting dissimilarity measure
   between g and ref_c = | \times I_{ref} - W_q \times I_q |
A_T= currently assigned cluster number
MinDism = dissimilarity measure between input
    sequence g and cluster A_T = S(g, ref_A)
H_c= threshold value of cluster c = W_{cmax} \times L_{cmax} \times 55\%
s_c = current size (number of sequences) of cluster c
avgval_x= average length per sequence of cluster x
      = total length of sequences
          total number of sequences
V_c = weighted-length of the cluster c
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= $\sum W_q \times I_q$, gene g in cluster c

PROPOSED ALGORITHM: RaTa (Method)

Input: String of sequences (FASTA format).Output: Clusters of sequences.

Begin

- 1. Initialize MinDism to INFINITY and A_T to 0
- 2. Assign weight w_i to each different element i of gene sequence in input database.
- 3. Make the first sequence as first cluster and mark it as reference gene of that cluster.
- 4. Calculate V_1 and H_2 according to definition.
- 5. When a new sequence *g* arrives

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5.1. For each cluster i

5.1.1. Find S(g, ref_i)

5.1.2. if S(g, ref_i) < H_i and S(g, ref_i) < Min_Dis

5.1.2.1. MinDism = S(g, ref_i)

5.1.2.2. A_T = i.

5.2. If A_T not equal to zero
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5.2.1. assign the sequence to cluster A_T

5.2.2. For cluster A_T 5.2.2.1. For new sequence g5.2.2.1.1. Calculate W_g 5.2.2.1.2. $temp1 = W_g \times I_g$ 5.2.2.1.3. $temp2 = V_{A_T} + temp1$ 5.2.2.1.4. $S_{A_T} = S_{A_T} + 1$ 5.2.2.1.5. $avgval_{A_T} = \frac{temp2}{S_{A_T}}$

5.2.2.1.7. find the sequence in the cluster whose gene value is closest to and make it reference gene sequence.

5.3. If A_T equal to zero

5.3.1. create a new cluster *d* and assign the sequence to it

5.3.2. make the sequence as reference gene

5.3.3. calculate V_d

5.3.4. $A_T = d$

6. Calculate H_{A_T}

7. MinDism = INFINITY, $A_T = 0$

8. Repeat steps 5 - 7 until all the available sequences are clustered.

END

REFERENCES

- 1. "Interactive clustering model for explanation of Genomic Data", www.cse.msstate.edu
- 2. D. Jiang, C. Tang, A. Zhang, "Cluster analysis for gene expression data: A survey", *IEEE Trans. Knowl. Data Eng.*, vol. 16, no. 11, pp. 1370-1386, Nov. 2004.

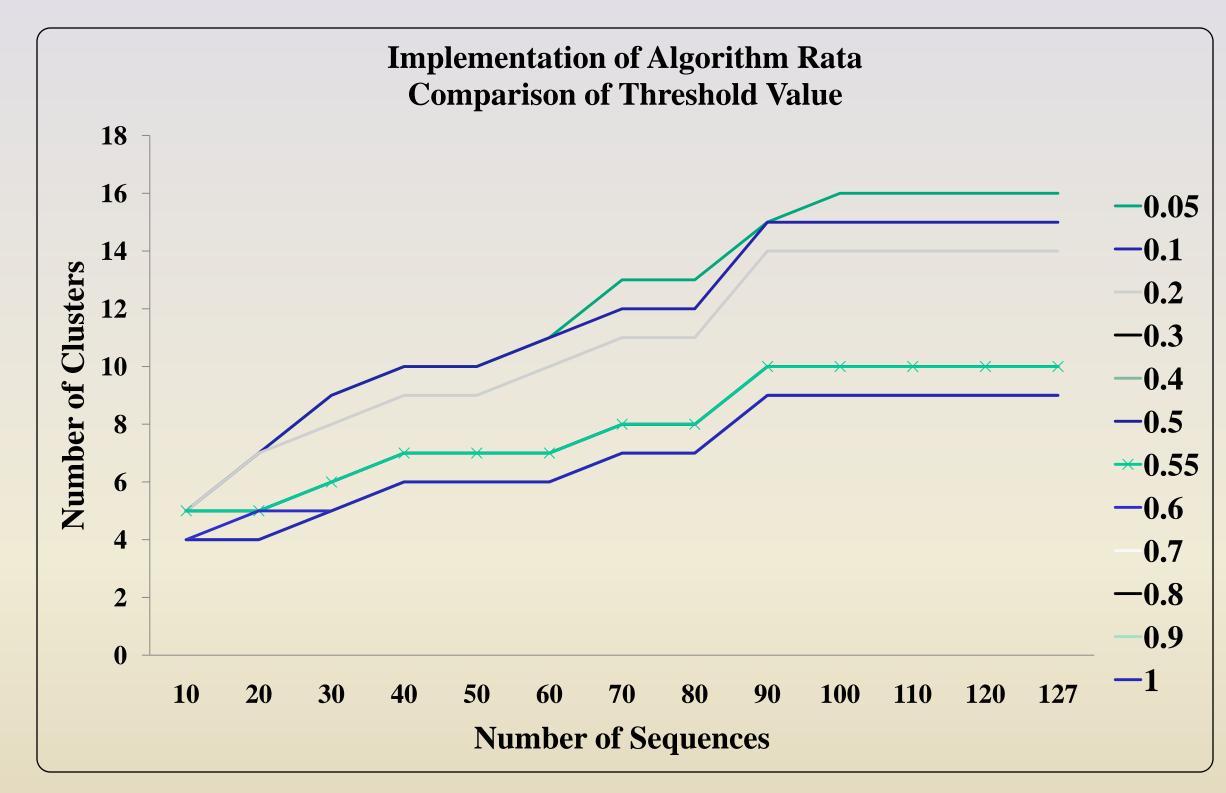
RESULTS & OBSERVATION

Space Complexity:

Here maximum possible number of clusters is n. Again the maximum possible gene sequences in a cluster are also n and the maximum length of each sequence is L. So, the space complexity is $O(n^2L)$.

Time Complexity:

Line (1-4) need O(1) time. Step 5 needs O(n) time. All other lines require constant time operation. So for n sequence, the total running time of the algorithm is O(n²).



Implementation of algorithm shows (see graph) number of cluster increases with number of sequences; But remains almost static at some stages. Curves are obtained by varying the values of the threshold value H from 0.05 to 1. Curve will be smooth based on number of input sequences and intervals. Marked line refer average threshold value 0.55, which mentioned in algorithm

Conclusion and Future Works

Algorithm output can be used as input for phylogenetic tree constructions

Future scope includes:

- 1. Inclusion of dynamic clustering
- 2. Proof of optimality of the algorithm in parallel computation

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