MC-Cons: RNA secondary structure assignments

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Abstract

RNA secondary structural assignment is an interesting problem. Bla bla bla.

Author Summary

Introduction

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$$D_{coll} = \frac{D_f + \frac{[S]^2}{K_D S_T} D_S}{1 + \frac{[S]^2}{K_D S_T}}, D_{sm} = \frac{D_f + \frac{[S]}{K_D} D_S}{1 + \frac{[S]}{K_D}}, \quad (1)$$

Methods

Simple Tree Distance for Secondary Structure

Base Pair Tree Representation RNA secondary structure can represented by base pair trees, where only base pairs are considered. This representation is very similar to level 3 RNA abstract shape [1], albeit the stem length information is conserved. Although this representation greatly increases the size of the auxiliary space (codomain) compared to level 3 abstract shapes, it doesn't suffer from major changes in representation if small stem-loops are added or removed. It also doesn't map structures of widely varying stem length to the same element in the codomain.
The mapping from a Vienna dot bracket representation can be made simply by removing the dots (unpaired nucleotides) and then creating a tree from it. Since all nodes represent base pairs, the resulting tree can be considered unlabelled. Note that an artificial root is added to all trees.

Unit Tree Indel Distance The unit tree indel distance is a simple and intuitive distance function based on the well known tree edit distance [2,3], where insertions and deletions have a unit cost. Since it is applied to base pair trees which are unlabelled, node relabelling comes at no cost.
Using this scoring scheme, a distance of n means that the smallest number of base pair breakage or formation to transition from a base pair tree to another is n. The distance function retains the metric properties.

Optimization goal

The idea of minimizing the sum of pairwise distance between sets of objects if far from new and a significant body of work has been done in the field of location theory [4].

MC-Cons

MC-Cons is a two-step optimization process relying on the minimization of the sum of pairwise distance of two distance functions. First, the

Metaheuristics

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1. react
2. diffuse free particles
3. increment time by dt and go to 1

Results

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IRES

Although IRES tend to fold in very similar shapes,

A more advanced level: tRNA alternative folding

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Discussion

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Supporting Information

S1 Video

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