

Progress in the Enumeration Approach to Computing Equilibrium of Interacting Nucleic Acid Strands

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DNA is one of the most promising material for constructing logical circuits, memory, intelligent devices equipped in molecular robots([1]). The problem of designing nucleic acid strands to avoid unwanted structures is difficult since they can form tremendously many number of structures and thus we need much of computation time for the analysis. Nucleic acid strand interaction analysis at equilibrium has been tackled by Dirks, et al.([2]), who have nicely extended McCaskill's partition function computation algorithm for a single RNA molecule ([3]) to the case of multiple strands, and furthermore succeeded in computing the equilibrium state of interacting RNA molecules by using convex programming after computing partition functions of all strand complexes. The author introduced a new general approach to computing chemical equilibrium based on graph theory and optimization theory([4][5]). Distinguished feature of the method was that it only used convex programming but not dynamic programming. Essential point of the method based on the idea of enumerating all the structures in a reaction system by using a graph. This method was applied also to nucleic acid strands interaction, where we considered only linear secondary structures([6]). In this poster presentation, we will present further progress of this approach to the analysis of interacting nucleic acid strands.

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