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Nucleic Acid Conformation Space as an Optimization Problem on Simultaneous Group Equations

Conformational changes in the phosphate backbones of individual nucleotides is a primary driver of large scale, polynucleotide conformational changes. As much of the functionality of RNA is derived from its conformation, thorough knowledge of the conformational limits of its constituent components is therefore of great importance. By viewing the phosphate backbone as a kinematic chain and sampling the chain's solution space in a regular manner, I demonstrate that the conformation space of a nucleotide backbone can be approximated by viewing the sample space as a graph edge cover problem with unusual conditions. By defining a group on the set of perfect matchings of bipartite graphs, the cover problem is reduced to finding a minimum solution to a system of group equations.