AN $O(n^5)$ ALGORITHM FOR MFE PREDICTION OF KISSING HAIRPINS AND 4-CHAINS IN NUCLEIC ACIDS

HO-LIN CHEN [1], ANNE CONDON [2], AND HOSNA JABBARI [2]
1 CALIFORNIA INSTITUTE OF TECHNOLOGY, CENTER FOR MATHEMATICS OF INFORMATION, HOLINC@GMAIL.COM
2 DEPARTMENT OF COMPUTER SCIENCE, UNIVERSITY OF BRITISH COLUMBIA, {CONDON,HJABBARI}@CS.UBC.CA

Our knowledge of the amazing variety of functions played by RNA molecules in the cell continues to expand, with the functions determined in part by structure. To improve our ability to determine function from DNA or RNA sequences, and also to aid in the design of nucleic acids with novel structural or functional properties, accurate and efficient structure prediction methods are valuable. Currently, computational methods focus mostly on secondary structure prediction. Of particular interest, from a computational standpoint, is prediction of pseudoknotted secondary structures.

A common approach to prediction of secondary structure from the base sequence is to find the minimum free energy (MFE)structure, from the possibly exponentially many structures. Since the general problem of MFE secondary structure prediction is NP-hard, polynomial-time algorithms handle a restricted class of secondary structures.

We present a novel MFE secondary structure prediction algorithm with respect to a thermodynamic model that encompasses the Turner model, which significantly expands the class of structures handled in $O(n^5)$ time. Our algorithm can handle biologically important examples including H-type pseudoknots, kissing hairpins (previously handled in $O(n^6)$ time), and chains of four pairwise overlapping stems, as well as nested substructures of these types (not handled by previous $O(n^5)$ algorithms).