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Finding folding and function prediction for non-coding RNA: A new comparative approach

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The available huge experimental sequence information calls for computational prediction methods for problems, such as RNA structure prediction, RNA-RNA interactions prediction, genomic scans for conserved RNA structural elements and RNA design. In our previous work on simultaneous alignment and folding of two sequences - the so-called Sankoff's problem - we have shown that classical alignment algorithm and hybridization without intra-molecular base-pairing are mathematically equivalent. In this work we complete the solution of Sankoff's problem showing how to include in the frame of classical alignment an algorithm for folding and co-folding. We present a model that integrates both the energy-based and evolutionary-based information of sequence/structure co-variations to predict the simultaneous folding/co-folding and alignment of RNA/DNA sequences, by constructing multi-structure (folding or co-folding)/sequence alignments from sequence comparisons. The combined evolutionary and thermodynamic partition function is computed by means of a dynamic programming algorithm and used to determine the probabilities of an alignment and folding/co-folding match between two sequence positions. For calculation of match probabilities detailed recursion relations for partition functions of alignments and folding/co-folding are based on their recursion analogs of subsequences. The partition function is used for backtracking and reconstructing a properly weighted ensemble of optimal and suboptimal multi-structure/sequence alignments. The model is tested on different data sets of non-coding RNA.

Biography

Roumen A Dimitrov earned his Doctorate in Computational Biology from Wageningen University, The Netherlands during 1997-2000. His multidisciplinary research experience includes works on: Electrostatic interactions in proteins as Research Scientist from Institute of Organic Chemistry, Bulgarian Academy of Sciences (1985-1990); physical basis of protein hierarchical organization as Post-graduate specialization on computational molecular biology from the Institute of Protein Researches, Pushino, Russia (1990-1994); and DNA and RNA partition function calculation as Postdoctoral Research Associate from Rensselaer Polytechnic Institute (2000 – 2004), USA. Currently he is a Lecturer at University of Sofia, Bulgaria.

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