A probabilistic approach to modeling RNA 3-D structure

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The prediction of macromolecular 3-D structure is one of the prime open problems in computational biology. In research the main focus has been on protein 3-D structure prediction. However, the prediction of non-coding RNA 3-D structure constitutes a relatively young and growing research field, as many new non-coding RNA molecules are being discovered these years and it is becoming evident that they play a more significant role in the cell than previously thought. Hence, methods for analyzing and sampling RNA 3-D structures are increasingly important.

Currently, the most common approach to modeling local RNA 3-D structure has been to describe the local conformational space as discrete in a non-probabilistic framework. We present an original approach to modeling local RNA 3-D structure using a probabilistic model that treats the conformational space as continuous. In our model the dihedral angles in RNA are modeled with a Dynamic Bayesian Network using directional statistics. The model defines a continuous probability distribution over the conformational space and therefore has numerous applications. It allows for fast probabilistic sampling of locally RNA-like structures and it can therefore be used in RNA 3-D structure prediction, where one of the problems is efficiently searching through the space of plausible RNA structures. The model is also well suited to be used in quality validation of experimentally determined structures.