Prediction of RNA secondary structure including pseudoknots for long sequences

Kengo Sato^{1,a)} Yuki Kato^{2,b)}

Abstract: RNA structural elements called pseudoknots are involved in various biological phenomena including ribosomal frameshifts. Because it is infeasible to construct an efficiently computable secondary structure model including pseudoknots, secondary structure prediction methods considering pseudoknots are not yet widely available. We developed IPknot, which uses heuristics to speed up computations, but it has remained difficult to apply it to long sequences because it requires cubic computational time with respect to sequence length and has threshold parameters that need to be manually adjusted. Here, we propose an improvement of IPknot that enables calculation in linear time by employing the LinearPartition model and automatically selects the optimal threshold parameters based on the pseudo-expected accuracy. IPknot showed favorable prediction accuracy across a wide range of conditions in our exhaustive benchmarking, not only for single sequences but also for multiple alignments.

Keywords: RNA secondary structure prediction, Pseudoknots, Integer programming

¹ Keio University, Yokohama, Kanagawa 223–8522, Japan ² Oseka Ujugriju, Suita Oseka 565, 0871, Japan

Osaka Uiversity, Suita, Osaka 565–0871, Japan
a) satoken@bio.keio.ac.in

a) satoken@bio.keio.ac.jp
b) wkato@rna.med.osaka.u.a

b) ykato@rna.med.osaka-u.ac.jp