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RNA structure characterization from chemical mapping experiments

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Despite great interest in solving RNA secondary structures due to their impact on function, it remains an open problem to determine structure from sequence. Among experimental approaches, a promising candidate is the "chemical modification strategy", which involves application of chemicals to RNA that are sensitive to structure and that result in modifications that can be assayed via sequencing technologies. One approach that can reveal paired nucleotides via chemical modification followed by sequencing is SHAPE, and it has been used in conjunction with capillary electrophoresis (SHAPE-CE) and high-throughput sequencing (SHAPE-Seq). The solution of mathematical inverse problems is needed to relate the sequence data to the modified sites, and a number of approaches have been previously suggested for SHAPE-CE, and separately for SHAPE-Seq analysis. Here we introduce a new model for inference of chemical modification experiments, whose formulation results in closed-form maximum likelihood estimates that can be easily applied to data. The model can be specialized to both SHAPE-CE and SHAPE-Seq, and therefore allows for a direct comparison of the two technologies. We then show that the extra information obtained with SHAPE-Seq but not with SHAPE-CE is valuable with respect to ML estimation.

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