DNA Computing Complexity Analysis Using DNA/DNA Hybridization Kinetics

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To solve more complex problems and to develop more efficient molecular algorithms, it is necessary to analyze the complexity of DNA computing. The complexity of any computational algorithm is typically measured in terms of time and space. In DNA computing, the time complexity can be measured by the total reaction time of the experiments and the time required for each operation, and the space complexity by the physical volume of the required molecules.

As a first step, we consider the case of perfect hybridization between two DNA strands (A and B) and one complement strand (e) which is denoted ($A \rightarrow_e B$). This situation can be regarded as a unit operation for the basic DNA computing algorithm. Then, the time and volume complexities of hybridization reaction are estimated. This can be considered as an initial-pool generation step for Adleman-style DNA computing algorithm for a simple two-node directed graph. Based on the calculated time and volume for the primitive operation, the complexity of DNA algorithm for the general n-node graph problem can be estimated.

Our analysis is based on the DNA/DNA hybridization reaction mechanism with chemical kinetic models. This research is the first approach to describe the worst case analysis of generate-and-filter DNA algorithm using a standard chemical kinetic equations with the kinetic constants (forward reaction kinetic constant, k, and reverse reaction kinetic constant, k_{-1}). Previous approaches are based on the classical algorithm analysis method or a simple kinetic model.

The analysis results will be helpful to understand the practical limitation of exhaustive DNA computing algorithms and to guide the setting of the lab protocols of DNA algorithms. Additionally, they will be useful to simulate DNA reaction processes such as hybridization, since it can determine the initial number of DNA molecules and total time in digital computer referred to the protocols of real lab experiments. We utilize the results for developing DNA computing simulator, NACST/Sim.[1]

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