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Molecular beacon computing model for maximum weight clique problem

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Abstract

Given an undirected graph with weights on the vertices, the maximum weight clique problem requires finding the clique of the graph which has the maximum weight. The problem is a general form of the maximum clique problem. In this paper, we encode weight of vertex into a unique fixed length oligonucleotide segment and employ sticker model to solve the problem. The proposed method has two distinct characteristics. On one hand, we skip generating initial data pool that contains every possible solution to the problem of interest, the key point of which is constructing the solution instead of searching solution in the vast initial data pool according to logic constraints. On the other hand, oligonucleotide segments are treated like variables which store weights on vertices, no matter what kind of number the weights are, integer or real. Therefore, the proposed method can solve the problem with arbitrary weight values and be applied to solve the other weight-related problem. In addition, molecular beacon is also employed in order to overcome shortcomings of sticker model. Besides, we have analyzed the proposed algorithm's feasibility.

Keywords: DNA computing; Maximum weight clique; Molecular beacon

1. Introduction

Molecular beacons are dual-labeled oligonucleotide probes that have a fluorescent dye (reporter) at one end and a fluorescence quencher (usually DABCYL) at the opposite end [10,11]. The probe is designed with a target-specific hybridization domain positioned centrally between short sequences that are self-complementary and are usually unrelated to the target sequence. In the absence of target, the self-complementary domains anneal to form a stem-loop hairpin structure in a unimolecular reaction that serves to bring the fluorescence reporter group into close proximity with the quencher group, and results in quenching of the reporter. In this configuration, the molecular beacon is 'dark' (Fig. 1a). Reporter-dye quenchers such as DABCYL and Black Hole Quencher (BHQ) work based on both fluorescence resonance energy transfer (FRET) and the formation of an exciton complex between the fluorophore and

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(a) In the absence of target sequence MB is 'dark'.

(b) In the presence of target sequence, MB is 'bright'.

Fig. 1. Schematic diagram of principle of MB.

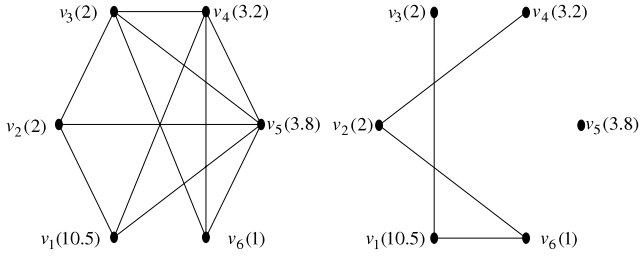

Fig. 2. A 6-vertex undirected graph with weights on vertices and its complement graph.

the quencher. Thus, DABCYL quenches the reporter dye only in the hairpin form partly due to its relatively short Forster radius. In the presence of target, the central loop domain will hybridize with the complementary target DNA or RNA in a bimolecular reaction, forcing the molecule to unfold; reporter and quencher are now physically separated and the fluorescence of the reporter dye will be restored upon excitation. In this configuration, the molecular beacon is 'bright' (see Fig. 1b).

The significant advantage of molecular beacon is that they can recognize target sequences with a greater degree of specificity than linear probes. Molecular beacons are readily capable of discriminating between targets that differ by only a single nucleotide. The reason is that the unimolecular hairpin reaction competes with bimolecular probe-target hybridization and serves to reduce the relative stability of undesired imperfect (mismatch) hybridization events. Thermodynamic analysis [1] of molecular beacon reveals that the range of temperatures within which discrimination between perfect matched target sequence and imperfect matched target sequence (even a single nucleotide is unmatched) is wider for molecular beacons than it is for the corresponding linear probes. This is the very reason that molecular beacon is capable of discriminating between targets that differ by only a single nucleotide.

The clear advantages of molecular beacons over linear oligonucleotide probes have led to their use in numerous applications ranging from quantitative PCR, to the study of protein–DNA interactions, to the visualization of RNA expression in living cells. Most recently, Yin [15] proposed DNA computing model for 3-SAT problem using molecular beacon, which has initialized a brand-new application field for the molecular beacon.

2. Maximum weight clique problem

Assume that $G = \{V, E, W\}$ is an undirected graph with weights on vertices, where V is the set of vertices and E is the set of edges, W is the weight vector, each component of W, denoted by $\omega_i (i = 1, 2, \ldots, n)$, is the weight of the ith vertex in the graph. Assume that ω_i is a positive real number. For arbitrary clique S of V, the weight of clique is defined as: $W(S) = \sum_{i \in S} \omega_i$. If $S = \Phi$, then $W(\Phi) = 0$. Fig. 2 shows a 6-vertex undirected graph with weight vector $W = (10.5, 2, 2, 3.2, 3.8, 1)^T$ and its complement graph.

The maximum weight clique problem requires finding the clique of the graph which has the maximum weight. Note here, the maximum weight clique is not necessarily the maximum clique in the graph. The problem is a general form of the maximum clique problem. It has been widely applied in pattern recognition and robot technique. The

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