



A new parallel algorithm to solve one classic water resources optimal allocation problem based on inspired computational model

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ABSTRACT

The shortage of freshwater resources is a serious problem in the process of urbanization in the world, and even become the main constraint factor in some areas. In order to solve the problem, it is imperative to develop an effective, flexible and low-cost water resources management plan. Water resources optimal allocation is one of the hot topics in the field of water resources at present, such as water resources optimal k -edge cover problem. The k -edge cover problem aims to find an edge cover set with k edges in a given undirected graph. The efficient solution of this problem can play an important role in planning and setting up urban water resources network sites. Based on DNA molecular computing, the paper use a new parallel algorithm to solve k -edge cover problem with $O(n^2)$ time complexity, which greatly simplifies the computing complexity.

Keywords: DNA computation; Water resources optimal allocation problem; The k -edge cover problem; Adleman-Lipton model; NP-complete problem

1. Introduction

The problem of water resources optimal allocation is theoretically a multi-objective stochastic sequential decision making problem. It is to utilize the effective, fair and sustainable principles, to allocate limited and different forms of water resources scientifically and reasonably through a variety of measures in a specific basin or area. The water resources optimal allocation is the basis of the water resources rational utilization and the fundamental guarantee for the water resources sustainable utilization.

In fact, the water resources rational allocation, in a broad sense, is a study of how to use good water resources,

including the development, utilization, protection and management of water resources. It is more urgent to carry out water resources rational allocation. The main reasons are as below: first, the natural spatial and temporal distribution of water resources does not adapt to the distribution of productive forces. Secondly, there have lots of water competitions between the regions and the various water use departments, and thirdly, the water resources development and utilization have caused many ecological environmental problems.

The rational allocation of water resources is a comprehensive system consisting of various measures. Its basic functions include two aspects: by adjusting the industrial structure, building a water-saving society, adjusting the

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distribution of productivity, restraining the momentum of water demand, and adapting to the more unfavorable conditions of water resources in demand, and coordinating competitive water use, strengthening management and changing water resources through engineering measures in the supply side. Natural space-time distribution is adapted to the distribution of productive forces. The two aspects complement each other in order to promote the sustainable development of the region. Rational allocation is the goal and desire when people allocate scarce resources. Generally speaking, the results of a reasonable allocation are not the best for the benefit or benefit of a certain individual, but the overall benefit or benefit of the whole resource allocation system is the best. The optimal allocation is the way and means people are looking for in reasonable allocation plan.

Since Adleman’s pioneering work in Hamilton path problem [1], the research about DNA parallel computing has undergone rapid development process. Because of its advantages with parallelism and storage efficiency features, DNA parallel computing has been used to solve optimization NP-complete problems [2–18]. DNA computing refers to the process of solving the problems by producing and detecting a combination of a kind of mathematical process, which is based on DNA molecules parallel biochemical operations and processing techniques.

In general, DNA computing has three steps: (1) Generate DNA molecular data pools representing all possible solutions to the unsolved problem; (2) a series of biochemical experiments are carried out to eliminate the DNA solution chains which do not meet the logical requirements of the problem; (3) select the optimal solution chains for the problem. At present, DNA computing research involves many aspects, such as DNA computing capability, models and algorithms.

The k -edge cover problem, aiming to find the cover set with k edges, is a typical NP problem. For $G = (V,E)$, an edge cover means an edge set S of G such that $\forall v_i \in V$, then have at least one $e_{ij} \in S$ linking the vertex v_i . The k -edge cover problem is to find edge cover sets with k edges. For example, the undirected graph G in Fig. 1 is such a problem. There has no efficient algorithm to solve the problem by now. Based on the research of Adleman [1] and Lipton [2], we use a new bio-computing procedure to get the solutions of the k -edge cover problem.

The rest of the article is arranged as below. In the Section 2, we introduce the DNA computing Adleman-Lipton model and use the DNA molecular algorithm to solve k -edge coverage problem. Next, we describe feasibility and

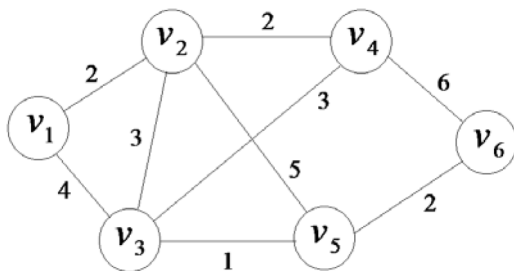


Fig. 1. An undirected graph G with 6 vertices and 9 edges.

complexity of the algorithm in Section 3. Then, experimental results of simulated DNA computing are shown in Section 4. We come to the conclusion in Section 5.

2. DNA computing and DNA algorithm for the k -edge cover problem

Although biology and mathematics have their own complexity, in recent years, Mathematical Biology, as an interdisciplinary subject, has been intersecting from the two major fields of biology and mathematics. The operations in Adleman-Lipton model mainly include: *Merge* (T_1, T_2), *Copy* (T_1, T_2), *Separation* (T_1, L, T_2), *Discard* (T), *Read* (T), *Sort* (T_1, T_2, T_3) and *Append-tail* (T, y) [19–22]. Meanwhile, the complexity of these operations is $O(1)$ [23–25].

The symbols $1, A_k, B_k$ ($k = 1, 2, \dots, n$) denote distinct DNA singled strands with same length, say t -mer. We use distinct DNA singled strands $A_i B_j$ ($1 \leq i < j \leq n$) to denote the edge e_{ij} with $A_i B_j$ for e_{ij} including in the edge set. In order to get the optimum solutions, we meantime design weight information string X with t -mer length, that the number of pasting is determined by the weight w_{ij} of the edge e_{ij} . We use adjacency matrix of graph G denoting the connection relationship between different vertices, which $a_{ij} = 1$ means vertex v_i links with v_j and $a_{ij} = 0$ denotes connectionless. Taking Fig. 1 for example, the adjacency matrix $M(G)$ is as follows:

$$M(G) = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \end{bmatrix} \quad (1)$$

As the simple undirected graph has no self-loops, so $a_{ii} = 0$ and $a_{ij} = a_{ji}$. In progress, we only need to check the numerical value of upper triangular matrix $M(G)$. Let $T_1 = \{\emptyset\}$.

- (1) Generate all vertex set strands of graph G .
 For $i = 1$ to $i = n - 1$
 For $j = i + 1$ to $j = n$
 (1-1) If ($a_{ij} = 1$)
 Then
 (1-2) *Copy* (T_1, T_2);
 (1-3) *Append-tail* ($T_2, A_i B_j$);
 (1-4) *Merge* (T_1, T_2);
 (1-5) *Discard* (T_2);
 Else
 (1-6) Continue
 End for
 End for
- (2) Each single chain in the tube T_1 represents a possible set of edges after algorithm (1). As k -edge cover problem requires the edge cover set should contain k edges. So we pick out these strands with the $3kt$ -mer length since we denote each edge as $3t$ -mer length.
 (2-1) *Selection* ($T_1, 3kt, T_3$).

(3) Every singled chain in tube T_3 denotes a possible k edges set so far. Meanwhile, the edge cover problem requires that arbitrary vertex should connect at least one edge of set. Therefore, we should check whether all sets satisfy the constraints. For $\forall v_i \in V$ in graph, we should keep the strands with edge symbols A_i1 and $1B_i$ synchronously.

For $i = 1$ to $i = n$

- (3-1) Copy (T_3, T_4);
- (3-2) Separation ($T_3, \{A_i1\}, T_5$);
- (3-3) Separation ($T_4, \{1B_i\}, T_6$);
- (3-4) Merge (T_5, T_6);
- (3-5) Copy (T_5, T_3);
- (3-6) Discard (T_4);
- (3-7) Discard (T_5);
- (3-8) Discard (T_6).

End for

(4) The k -edge cover problem should be an edge cover set with minimum weight value. If edge e_{ij} in the edge cover set, we append additional weight strand X with w_{ij} times in order to get the corresponding strand solutions.

For $i = 1$ to $i = n - 1$

For $j = i + 1$ to $j = n$

- (4-1) Separation ($T_3, \{A_i1B_j\}, T_7$);
- (4-2) Append-tail ($T_7, XX...X$);
- (4-3) Merge (T_3, T_7);
- (4-4) Discard (T_7).

End for

End for

(5) We find the shortest DNA chains by sorting, which indicate the optimal solutions of the problem.

- (5-1) Sort (T_3, T_8, T_9);
- (5-2) Read (T_8).

3. The complexity and feasibility of the proposed DNA algorithm

3.1. Theorem

The solutions of k -edge cover problem having n vertices can be got in $O(n^2)$ time complexity by biological molecules parallel computing.

3.2. Proof

We first generate arbitrary edges sets strands in T_1 at Algorithm (1). Then, after Algorithm (2), all the singled strands in tube T_3 denote all possible k -edges set. Then the strands can be described:

$$A_{i_1}1B_{j_1}A_{i_2}1B_{j_2}...A_{i_k}1B_{j_k} \quad i_k, j_k \in \{1, 2, \dots, n\} \quad (2)$$

Next, we choose the edge cover set strands and append the weight strands at the end of corresponding strands at Algorithm (3) and Algorithm (4). S can be supposed as the strands after the Algorithm (4). Then they can be described:

$$A_{i_1}1B_{j_1}A_{i_2}1B_{j_2}...A_{i_k}1B_{j_k}XX...XX \quad (3)$$

And we reasonably design the length of $A_{i_p}B_{j_p}1$ and X , for $\|A_k\| = \|B_k\| = \|1\| = \|\#\| = t$. We suppose $\max(w_{i_pj_p}) = L$, so

$$\begin{aligned} \|S\| &= \|A_{i_1}\| + \|1\| + \|B_{j_1}\| + \|A_{i_2}\| + \|1\| + \|B_{j_2}\| + \\ &\dots + \|A_{i_k}\| + \|1\| + \|B_{j_k}\| + \|X\| + \dots + \|X\| = \\ &\sum_{p=1}^k \|A_{i_p}\| + \sum_{p=1}^k \|1\| + \sum_{p=1}^k \|B_{j_p}\| + (w_{i_1j_1} + w_{i_2j_2} + \dots + w_{i_kj_k})t \end{aligned} \quad (4)$$

$$= 3kt + (w_{i_1j_1} + w_{i_2j_2} + \dots + w_{i_kj_k})t$$

$$\max(w_{i_pj_p}) = L \quad (5)$$

$$3kt \leq \|S\| \leq 3kt + kL \quad (6)$$

So the solutions strands of Algorithm (5) can be found in appropriate length range between $3kt$ and $3kt + kL$.

In addition, the calculation of DNA algorithm time complexity T is as below:

$$\begin{aligned} T(\text{Algorithm (1)}) &= O(6n(n-1)/2) = O(n^2); \\ T(\text{Algorithm (2)}) &= O(1); \\ T(\text{Algorithm (3)}) &= O(8n) = O(n); \\ T(\text{Algorithm (4)}) &= O(4n(n-1)/2) = O(n^2); \\ T(\text{Algorithm (5)}) &= O(2) = O(1); \\ T &= T(\text{Algorithm (1)}) + T(\text{Algorithm (2)}) + T(\text{Algorithm (3)}) \\ &\quad + T(\text{Algorithm (4)}) + T(\text{Algorithm (5)}) \\ &= O(n^2) + O(1) + O(n) + O(n^2) + O(1) \\ &= O(n^2) \end{aligned}$$

4. Experimental results of simulated DNA computing

DNA-based calculations depend on the biochemical operations of molecules, which may lead to errors in the application of these biochemical operations. Therefore, how to design DNA sequences is an important issue to ensure the reliability of DNA computation. In order to make good performance in hybridization reactions, we learn from the sequence design methods in reference [34–40].

In this paper, we use BioPython, a computational molecular biology tool, as our development platform to generate good DNA sequences suitable for performing our algorithms in the laboratory. The Braich's programs run on Windows XP systems, with Intel kernel CPU and 8 GB main memory, and Visual C++ compiler. The coding programs are used to generate DNA sequences for solving the k -edge cover problem, and construct the DNA sequences of each bit in the library. Meanwhile, when a new DNA sequence is added, the program determines whether the DNA strand meets the constraints listed in the reference [34–41]. If the generated DNA sequence cannot satisfy the constraints, the program will regenerate the new DNA sequence. If the restriction condition is satisfied, the DNA sequence is accepted. When all DNA strands satisfy these constraints, the program stops, and these sequences are the output.

Taking 3-edge cover problem in Fig. 1 for an example, the program generates 4-base random sequences, consisting of $A, B, 1$ and X shown in Table 1. Edge DNA sequences

Table 1
Sequences chosen to represent $A_i, B_i, 1$ and $X (i \in \{1,2,\dots,6\})$ for the 3-edge cover problem

Bit	3'-5'DNA sequence	Bit	3'-5'DNA sequence
A_1	AGAT	B_1	CGCA
A_2	TGAT	B_2	ATTG
A_3	GTGT	B_3	TCTG
A_4	TGAG	B_4	GGCT
A_5	AGCG	B_5	CAGT
A_6	TGCT	B_6	AGTC
1	GACA	X	CCTA

generated by Braich's program are shown in Table 2. And we also calculate the enthalpy, entropy, and free energy for binding of each probe to its corresponding region on a library strand using the Braich's program, while the energy used is shown in Table 3.

We also calculate the mean and standard deviation of enthalpy, entropy and free energy in all probe/library inter-

Table 2
Sequences chosen to represent the elements $A_i1B_j (1 \leq i < j \leq 6)$ for the 3-edge cover problem

Bit	3'-5'DNA sequence	Bit	3'-5'DNA sequence
$A_{11}B_2$	AGATGACAATTG	$A_{11}B_3$	AGATGACATCTG
$A_{21}B_3$	TGATGACATCTG	$A_{21}B_4$	TGATGACAGGCT
$A_{21}B_5$	TGATGACACAGT	$A_{31}B_4$	GTGTGACAGGCT
$A_{31}B_5$	GTGTGACACAGT	$A_{41}B_6$	TGAGGACAAGTC
A_51B_6	AGCGGACAAGTC		

Table 3
The energies for of binding each probe to its corresponding region on a library strand

Edges	Enthalpy energy H	Entropy energy S	Free energy G
$A_{11}B_2$	108.7	278.5	24.6
$A_{11}B_3$	104.6	267.7	23.1
$A_{21}B_3$	103.5	261.2	22.7
$A_{21}B_4$	101.3	254.3	22.3
$A_{21}B_5$	107.4	270.1	24.5
$A_{31}B_4$	99.7	250.6	23.3
$A_{31}B_5$	105.8	270.8	23.9
$A_{41}B_6$	107.1	272.4	24.2
$A_{51}B_6$	102.2	261.8	22.8

Table 5
DNA sequences chosen to represent the solutions to the 3-edgecover problem in Fig. 1

e_{ij}	$e_{12'}e_{34'}e_{56}$
Solutions strands	3'-AGATGACAATTGGTGTGACAGGCTAGCGGACAAGTCCCCTACCTACCTACCTACCTACCTA-5'

Table 4
The energies over all probe/library strand interactions

	Enthalpy energy H	Entropy energy S	Free energy G
Average	104.478	265.267	23.489
Standard Deviation	3.0429	9.0128	0.8388

actions. The energy level is shown in Table 4. Table 5 gets solutions strands of the 3-edge cover problem.

5. Conclusions

This paper introduces a new DNA computing algorithm to solve k -edge cover problem. The DNA algorithm has two merits. First of all, the aforementioned algorithm has a lower hybrid error rate, as we utilize reasonable DNA sequences to produce solutions. Secondly, the DNA algorithm can deal with the k -edge cover problem having n vertices in the $O(n^2)$ time complexity and compare exponential time complexity with the electronic computer, such as $2^{O(k)n^{O(1)}}$ [29], $O(2.3147^k)$ [30], $O(n^3)$ [32] and so on. Many scholars believe that the study of DNA computing lays the foundation for human development of molecular computers. The intelligent system based on DNA computing will set up a bridge between DNA computing and intelligent system research, and will play a stepping stone role in DNA intelligent computers and other related research. The integration of DNA computing and soft computing will provide a good method to realize DNA intelligent computers. DNA intelligent computer can completely solve the intelligent computing function that the existing computer can't achieve [26–28].

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