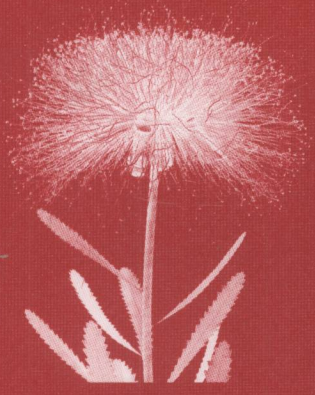
Carlos Cotta
Jano van Hemert (Eds.)

Evolutionary Computation in Combinatorial Optimization

LNCS 4446

7th European Conference, EvoCOP 2007
Valencia, Spain, April 2007
Proceedings



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Preface

Metaheuristics have often been shown to be effective for difficult combinatorial optimization problems appearing in various industrial, economical, and scientific domains. Prominent examples of metaheuristics are evolutionary algorithms, simulated annealing, tabu search, scatter search, memetic algorithms, variable neighborhood search, iterated local search, greedy randomized adaptive search procedures, estimation of distribution algorithms, and ant colony optimization. Successfully solved problems include scheduling, timetabling, network design, transportation and distribution, vehicle routing, the traveling salesman problem, satisfiability, packing and cutting, and general mixed integer programming.

EvoCOP began in 2001 and has been held annually since then. It was the first event specifically dedicated to the application of evolutionary computation and related methods to combinatorial optimization problems. Originally held as a workshop, EvoCOP became a conference in 2004. The events gave researchers an excellent opportunity to present their latest research and to discuss current developments and applications as well as providing for improved interaction between members of this scientific community. Following the general trend of hybrid metaheuristics and diminishing boundaries between the different classes of metaheuristics, EvoCOP has broadened its scope over the last years and invited submissions on any kind of metaheuristic for combinatorial optimization.

This volume contains the proceedings of EvoCOP 2007, the seventh European Conference on Evolutionary Computation in Combinatorial Optimization. It was held in Valencia, Spain, April 11–13, 2007, jointly with EuroGP 2007, the Tenth European Conference on Genetic Programming, EvoBIO 2007, the Fifth European Conference on Evolutionary Computation and Machine Learning in Bioinformatics, and EvoWorkshops 2007, which consisted of the following seven individual workshops: EvoCOMNET, the Fourth European Workshop on the Application of Nature-Inspired Techniques to Telecommunication Networks and Other Connected Systems; EvoFIN, the First European Workshop on Evolutionary Computation in Finance and Economics; EvoIASP, the Ninth European Workshop on Evolutionary Computation in Image Analysis and Signal Processing; EvoInteraction, the Second European Workshop on Interactive Evolution and Humanized Computational Intelligence; EvoMUSART, the Fifth European Workshop on Evolutionary Music and Art; EvoSTOC, the Fourth European Workshop on Evolutionary Algorithms in Stochastic and Dynamic Environments, and EvoTransLog, the First European Workshop on Evolutionary Computation in Transportation and Logistics. Since 2007, all these events are grouped under the collective name EvoStar, and constitute Europe's premier co-located meetings on evolutionary computation.

Accepted papers of previous EvoCOP editions were published by Springer in the series *Lecture Notes in Computer Science* (LNCS – Volumes 2037, 2279, 2611, 3004, 3448, and 3906).

EvoCOP	Submitted	Accepted	Acceptance ratio
2001	31	23	74.2%
2002	32	18	56.3%
2003	39	19	48.7%
2004	86	23	26.7%
2005	66	24	36.4%
2006	77	24	31.2%
2007	81	21	25.9%

The rigorous, double-blind reviewing process of EvoCOP 2007 resulted in a strong selection among the submitted papers; the acceptance rate was 25.9%. Each paper was reviewed by at least three members of the International Program Committee. All accepted papers were presented orally at the conference and are included in this proceedings volume. We would like to credit the members of our Program Committee, to whom we are very grateful for their quick and thorough work and the valuable advice on how to improve papers for the final publication. EvoCOP 2007 contributions deal with representations, heuristics, analysis of problem structures, and comparisons of algorithms. The list of studied combinatorial optimization problems includes prominent examples like graph coloring, knapsack problems, the traveling salesperson problem, scheduling, as well as specific real-world problems.

We would like to express our sincere gratitude to the internationally renowned invited speakers who gave the keynote talks at the conference: Ricard V. Solé, head of the Complex Systems Lab at the University Pompeu Fabra, Chris Adami, head of the Digital Life Lab at the California Institute of Technology, and Alan Bundy, from the Centre for Intelligent Systems and their Applications, School of Informatics at the University of Edinburgh.

The success of the conference resulted from the input of many people, to whom we would like to express our appreciation. We thank Marc Schoenauer for providing the Web-based conference management system. The local organizers, led by Anna Isabel Esparcia-Alcázar, did an extraordinary job for which we are very grateful. We thank the Universidad Politécnica de Valencia, Spain, for their institutional and financial support and for providing premises and administrative assistance, the Instituto Tecnológico de Informática in Valencia for cooperation and help with local arrangements, and the Spanish Ministerio de Educación y Ciencia for their financial support. Thanks are also due to Jennifer Willies and the Centre for Emergent Computing at Napier University in Edinburgh, Scotland, for administrative support and event coordination. Last, but not least, we would especially like to thank Jens Gottlieb and Günther Raidl for their support and guidance, to whom we owe a lot. From their hard work and dedication, EvoCOP 2007 has now become one of the reference events in evolutionary computation.

April 2007

Carlos Cotta
Jano van Hemert

Organization

EvoCOP 2007 was organized jointly with EuroGP 2007, EvoBIO 2007, and EvoWorkshops 2007.

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Table of Contents

A New Local Search Algorithm for the DNA Fragment Assembly Problem

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Abstract. In this paper we propose and study the behavior of a new heuristic algorithm for the DNA fragment assembly problem: PALS. The DNA fragment assembly is a problem to be solved in the early phases of the genome project and thus is very important since the other steps depend on its accuracy. This is an NP-hard combinatorial optimization problem which is growing in importance and complexity as more research centers become involved on sequencing new genomes. Various heuristics, including genetic algorithms, have been designed for solving the fragment assembly problem, but since this problem is a crucial part of any sequencing project, better assemblers are needed. Our proposal is a very efficient assembler that allows to find optimal solutions for large instances of this problem, considerably faster than its competitors and with high accuracy.

1 Introduction

With the advance of computational science, bioinformatics has become more and more attractive to researchers in the field of computational biology. Genomic data analysis using computational approaches is very popular as well. The primary goal of a genomic project is to determine the complete sequence of the genome and its genetic contents. Thus, a genome project is accomplished in two steps, the first one is the genome sequencing and the second one is the genome annotation (i.e., the process of identifying the boundaries between genes and other features in raw DNA sequence).

In this paper, we focus on the genome sequencing, which is also known as the DNA fragment assembly problem. The fragment assembly occurs in the very beginning of the process and therefor other steps depend on its accuracy. At present, DNA sequences that are longer than 600 base-pairs (bps) cannot routinely be sequenced accurately. For example, human DNA is about 3.2 billion nucleotides in length and cannot be read at once. Hence, large strands of DNA need to be broken into small fragments for sequencing in a process called *shotgun sequencing*. In this approach, several copies of a portion of DNA are each broken into many segments short enough to be sequenced automatically by machine. But this process does not keep neither the ordering of the fragments nor the

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portion from which a particular fragment came. This leads to the DNA fragment assembly problem [1] in which these short sequences have to be reassembled to their (supposed) original form. The automation allows shotgun sequencing to proceed far faster than traditional methods. But comparing all the tiny pieces and matching up the overlaps requires massive computation.

The assembly problem is therefore a combinatorial optimization problem that, even in the absence of noise, is NP-hard: given k fragments, there are $2^k k!$ possible combinations. Over the past decade a number of fragment assembly packages have been developed and used to sequence different organisms. The most popular packages are PHRAP [2], TIGR assembler [3], STROLL [4], CAP3 [5], Celera assembler [6], and EULER [7]. These packages deal with the previously described challenges to different extents, but none of them solves all of them. Each package automates fragment assembly using a variety of algorithms. The most popular techniques are greedy-based while other approaches have tackled the problem with metaheuristics [8]. This work reports on the design and implementation of a new problem aware local search algorithm to find fast and accurate solutions for large instances of the DNA fragment assembly problem. We additionally study the behavior of several variants of the basic method. Finally, we also compare the results of our approach with the ones of classical (real world) assemblers in order to test the actual interest of our method.

The remainder of this paper is organized as follows. In the next section, we present background information about the DNA fragment assembly problem. In Section 3, the details of our proposed heuristic are presented. We analyze the results of our experiments in Section 4. Finally, we end this paper by giving our final thoughts and conclusions in Section 5.

2 The DNA Fragment Assembly Problem

In order to determine the function of specific genes, scientists have learned to read the sequence of nucleotides comprising a DNA sequence in a process called DNA sequencing. To do that, multiple exact copies of the original DNA sequence are made. Each copy is then cut into short fragments at random positions. These are the first three steps depicted in Fig. 1 and they take place in the laboratory. After the fragment set is obtained, a traditional assemble approach is followed in this order: overlap, layout, and then consensus. To ensure that enough fragments overlap, the reading of fragments continues until a coverage is satisfied. These steps are the last three ones in Fig. 1. In what follows, we give a brief description of each of the three phases, namely overlap, layout, and consensus.

Overlap Phase - Finding the overlapping fragments. This phase consists of finding the best or longest match between the suffix of one sequence and the prefix of another. In this step, we compare all possible pairs of fragments to determine their similarity. Usually, a dynamic programming algorithm applied to semiglobal alignment is used in this step. The intuition behind finding the pairwise overlap is that fragments with a significant overlap score are very likely next to each other in the target sequence.

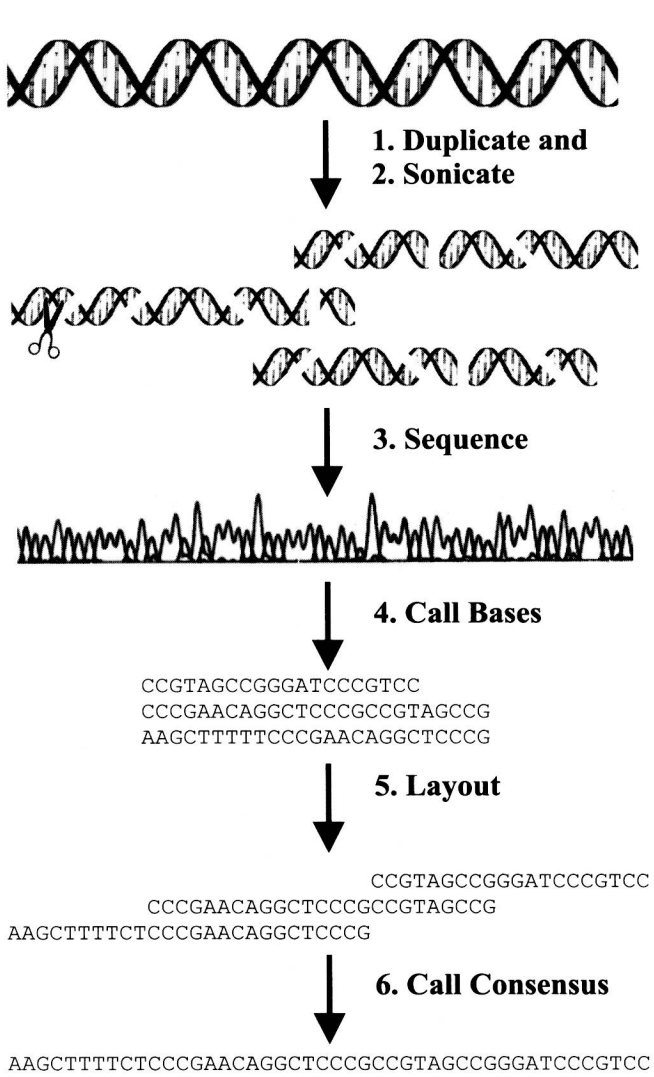

Fig. 1. Graphical representation of DNA sequencing and assembly

Layout Phase - Finding the order of fragments based on the computed similarity score. This is the most difficult step because it is hard to tell the true overlap due to the following challenges:

1. Unknown orientation: After the original sequence is cut into many fragments, the orientation is lost. One does not know which strand should be selected. If one fragment does not have any overlap with another, it is still possible that its reverse complement might have such an overlap.

2. Base call errors: There are three types of base call errors: substitution, insertion, and deletion errors. They occur due to experimental errors in the electrophoresis procedure (the method used in the laboratories to read the ADN sequences). Errors affect the detection of fragment overlaps. Hence, the consensus determination requires multiple alignments in highly coverage regions.
3. Incomplete coverage: It happens when the algorithm is not able to assemble a given set of fragments into a single contig. A contig is a sequence in which the overlap between adjacent fragments is greater or equal to a predefined threshold (cutoff parameter).
4. Repeated regions: "Repeats" are sequences that appear two or more times in the target DNA. Repeated regions have caused problems in many genome-sequencing projects, and none of the current assembly programs can handle them perfectly.
5. Chimeras and contamination: Chimeras arise when two fragments that are not adjacent or overlapping on the target molecule join together into one fragment. Contamination occurs due to the incomplete purification of the fragment from the vector DNA.

After the order is determined, the progressive alignment algorithm is applied to combine all the pairwise alignments obtained in the overlap phase.

Consensus Phase - Deriving the DNA sequence from the layout. The most common technique used in this phase is to apply the majority rule in building the consensus.

To measure the quality of a consensus, we can look at the distribution of the coverage. Coverage at a base position is defined as the number of fragments at that position. It is a measure of the redundancy of the fragment data, and it denotes the number of fragments, on average, in which a given nucleotide in the target DNA is expected to appear. It is computed as the number of bases read from fragments over the length of the target DNA [1].

$$Coverage = \frac{\sum_{i=1}^{n} length\ of\ the\ fragment\ i}{target\ sequence\ length} \tag{1}$$

where n is the number of fragments. The higher the coverage, the fewer number of the gaps, and the better the result.

3 Our Proposal: Problem Aware Local Search (PALS)

Classical assemblers use fitness functions that favor solutions in which strong overlap occurs between adjacent fragments in the layouts, using equations like 2 [9] (where $w_{i,j}$ is the overlap between fragments i and j). But the actual objective is to obtain an order of the fragments that minimizes the number of contigs, with the goal of reaching one single contig, i.e., a complete DNA sequence composed of all the overlapping fragments. Therefore, the number of contigs is used as a