

# On the Convergence of Chemical Reaction Optimization for Combinatorial Optimization

Albert Y.S. Lam, Victor O.K. Li, and Jin Xu

**Abstract**—A novel general-purpose optimization method, Chemical Reaction Optimization (CRO), is a population-based metaheuristic inspired by the phenomenon of interactions between molecules in a chemical reaction process. CRO has demonstrated its competitive edge over existing methods in solving many real-world problems. However, so far all studies concerning CRO are empirical in nature and no theoretical analysis has been conducted to study its convergence properties. In this paper, we present some convergence results for several generic versions of CRO, each of which adopts different combinations of the elementary reactions. We investigate the limiting behavior of CRO. By modeling CRO as a finite absorbing Markov chain, we show that CRO converges to a global optimum solution with probability arbitrarily close to one when time tends to infinity. Our results also show that the convergence of CRO is determined by both the elementary reactions and the total energy of the system. Moreover, we also study and discuss the finite time behavior of CRO.

**Index Terms**—Chemical reaction optimization, convergence, finite absorbing Markov chain, convergence rate, first hitting time.

## I. INTRODUCTION

CHEMICAL Reaction Optimization (CRO), as introduced in [1], is a recently proposed metaheuristic for combinatorial optimization problems. CRO loosely mimics the interactions of molecules in a chemical reaction, based on the principle that reactions yield products with the lowest energy on the potential energy surface (PES). CRO has demonstrated its splendid performance in solving many real-world optimization problems, e.g., spectrum allocation in cognitive radio systems [2], population transition in peer-to-peer live streaming [3], and task scheduling in grid computing [4]. Recently, it has also been applied to non-convex continuous problems [5]. For more information about the state-of-the-art development of CRO, the interested reader may refer to [6].

In this paper we focus on the combinatorial optimization problems, whose solution space is discrete, usually large, and finite. In general, a combinatorial optimization problem can be described as:

$$\min \{C(x) | x \in \mathcal{X}\}, \quad (1)$$

where  $\mathcal{X} \subset \mathbb{R}^N$  is the set of feasible solutions in the  $N$ -dimensional real number space,  $C(x) : \mathcal{X} \rightarrow \mathcal{Y} \subset \mathbb{R}$  is the cost function, and  $N$  is the dimension of the problem. Space  $\mathcal{X}$  is constructed according to all the constraints imposed on

the problem. Our goal is to find an optimal solution  $x^*$  in  $\mathcal{X}$ , which minimizes the cost function value such that  $C(x^*) \leq C(x)$  for all  $x \in \mathcal{X}$ . Without loss of generality, we assume that  $0 < C(x) < \infty$  for all  $x \in \mathcal{X}^1$ , which can be easily satisfied by adding a sufficiently large number to the objective function to construct a positive  $C(x)$ . In this way,  $C(x)$  can be viewed as the potential energy (PE) of the molecules in CRO.

Many theoretical analyses have been conducted to study the convergence of other popular evolutionary algorithms, e.g., Genetic Algorithm (GA) [8]–[10], Simulated Annealing (SA) [11], Ant Colony Optimization (ACO) [12]–[15], Threshold Accepting (TA) [16], etc. By using the homogeneous Markov chain, [10] shows that the canonical GAs with proportional selection will never converge to the global optimum, while its elitist variants do. [11] proves that given a sufficiently large number of iterations at each temperature, SA converges almost surely to the global optimum. [15] gives a short convergence proof for a class of ACO indicating that the probability of finding an optimal solution tends to unity when the algorithm is allowed to run forever. [16] suggests that TA will converge to the global optimum provided that the corresponding version of SA does. This is proved under the fact that SA usually belongs to the convex hull of TA. On the other hand, studies regarding the finite time behavior of evolutionary algorithms (EAs) have attracted great attention. Rudolph in [17] summarizes some results on the limiting and finite time behavior of EAs. [18] gives a survey on the time complexity of EAs for combinatorial optimization developed in the recent decade. Moreover, the convergence rate and the expected first hitting time of EAs are also investigated in [19] and [20], respectively. However, those EAs discussed above belong to GA or its variants. In other words, only the finite time behavior of GA has been studied. To summarize, all these results explain why the corresponding algorithms work well in practice.

CRO has been applied to tackle various types of nondeterministic polynomial-time hard (NP-hard) problems. Simulation results show that CRO is very competitive in solving many real-world NP-hard problems. Although abundant experimental and empirical research has already been done on CRO, to the best of our knowledge, no theoretical work has been conducted to analyze the performance of CRO. It is important to study the convergence properties of CRO; these properties allow a better understanding of the algorithm and facilitate

A.Y.S. Lam is with the Department of Computer Science, Hong Kong Baptist University, Kowloon Tong, Kowloon, Hong Kong. Email: albertlam@hkbu.org.

V.O.K. Li and J. Xu are with the Department of Electrical and Electronic Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong. Email: {vli, xujin}@eee.hku.hk.

<sup>1</sup>Any solution with infinite objective function value is considered as an infeasible solution [7]. The issue of non-negativity has been discussed in details in [5]. Here we make a stronger assumption of precluding the zero objective function value.

# Combinatorial Optimization And Empirical Processes Tinbergen Institute Research No 5

**Panos M. Pardalos, Ding-Zhu  
Du, Ronald L. Graham**



## **Combinatorial Optimization And Empirical Processes Tinbergen Institute Research No 5:**

**Combinatorial Optimization and Empirical Processes** Nanda Piersma, 1993 Combinatorial optimization problems involve an optimal choice from a countable set of alternatives Mathematical models for these problems are considered from a probabilistic point of view The aim of this research is to explore the usefulness of empirical process theory in the probabilistic analysis of combinatorial optimization problems This study shows that empirical process theory provides the probabilistic background to establish new results on the solution value of these problems such as gaussian tail bounds laws of the iterated logarithm and central limit theorems In line with the recent developments in this field probabilistic statements can be made for the solution value of arbitrary sized problems and not just for asymptotic values The applications include a wide range of combinatorial problems such as assignment covering and location problems **Management Science**, 2002 Issues for Feb 1965 Aug 1967 include Bulletin of the Institute of Management Sciences Books in Print, 1994 **Subject Guide to Books in Print**, 1975 **Forthcoming Books** Rose Arny, 1994-02 **Brinkman's catalogus van boeken en tijdschriften**, 1996 With 1901 1910 1956 1960 Repertorium is bound Brinkman's Titel catalogus van de gedurende 1901 1910 1956 1960 Title varies slightly *Boekblad*, 1994-04 **Edge-disjointness in Combinatorial Optimization** Jeroen de Kort, 1992 **Combinatorial Optimization** Mustafa Akgül, Horst W. Hamacher, Süleyman Tüfekci, 2012-12-06 There have been significant developments in the theory and practice of combinatorial optimization in the last 15 years This progress has been evidenced by a continuously increasing number of international and local conferences books and papers in this area This book is also another contribution to this burgeoning area of operations research and optimization This volume contains the contributions of the participants of the recent NATO Advanced Study Institute New Frontiers in the Theory and Practice of Combinatorial Optimization which was held at the campus of Bilkent University in Ankara Turkey July 16-29 1990 In this conference we brought many prominent researchers and young and promising scientists together to discuss current and future trends in the theory and practice of combinatorial optimization The Bilkent campus was an excellent environment for such an undertaking Being outside of Ankara the capital of Turkey Bilkent University gave the participants a great opportunity for exchanging ideas and discussing new theories and applications without much distraction One of the primary goals of NATO ASI is to bring together a group of scientists and research scientists primarily from the NATO countries for the dissemination of advanced scientific knowledge and the promotion of international contacts among scientists We believe that we accomplished this mission very successfully by bringing together 15 prominent lecturers and 45 promising young scientists from 12 countries in a university environment for 14 days of intense lectures presentations and discussions

*Combinatorial Optimization* Pierre Fouilhoux, Luis Eduardo Neves Gouveia, A. Ridha Mahjoub, Vangelis T. Paschos, 2014-07-21 This book constitutes the thoroughly refereed post conference proceedings of the Third International Symposium on Combinatorial Optimization ISCO 2014 held in Lisbon Portugal in March 2014 The 37 revised full papers

presented together with 64 short papers were carefully reviewed and selected from 97 submissions They present original research on all aspects of combinatorial optimization such as algorithms and complexity mathematical programming operations research stochastic optimization graphs and combinatorics

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Vangelis Th. Paschos, 2014-08-08 Combinatorial optimization is a multidisciplinary scientific area lying in the interface of three major scientific domains mathematics theoretical computer science and management The three volumes of the Combinatorial Optimization series aim to cover a wide range of topics in this area These topics also deal with fundamental notions and approaches as with several classical applications of combinatorial optimization Concepts of Combinatorial Optimization is divided into three parts On the complexity of combinatorial optimization problems presenting basics about worst case and randomized complexity Classical solution methods presenting the two most known methods for solving hard combinatorial optimization problems that are Branch and Bound and Dynamic Programming Elements from mathematical programming presenting fundamentals from mathematical programming based methods that are in the heart of Operations Research since the origins of this field

**Combinatorial Optimization** Bernhard Korte, Jens Vygen, 2018-03-13 This comprehensive textbook on combinatorial optimization places special emphasis on theoretical results and algorithms with provably good performance in contrast to heuristics It is based on numerous courses on combinatorial optimization and specialized topics mostly at graduate level This book reviews the fundamentals covers the classical topics paths flows matching matroids NP completeness approximation algorithms in detail and proceeds to advanced and recent topics some of which have not appeared in a textbook before Throughout it contains complete but concise proofs and also provides numerous exercises and references This sixth edition has again been updated revised and significantly extended Among other additions there are new sections on shallow light trees submodular function maximization smoothed analysis of the knapsack problem the  $\ln 4$  approximation for Steiner trees and the VPN theorem Thus this book continues to represent the state of the art of combinatorial optimization

Tenth EURO Summer Institute Combinatorial Optimization Summer Institute Combinatorial Optimization. 1994, Jouy-en-Josas, 1995

### **Handbook of Combinatorial Optimization**

Panos M. Pardalos, Ding-Zhu Du, Ronald L. Graham, 2013-09-07 The second edition of this 5 volume handbook is intended to be a basic yet comprehensive reference work in combinatorial optimization that will benefit newcomers and researchers for years to come This multi volume work deals with several algorithmic approaches for discrete problems as well as with many combinatorial problems The editors have brought together almost every aspect of this enormous field of combinatorial optimization an area of research at the intersection of applied mathematics computer science and operations research and which overlaps with many other areas such as computation complexity computational biology VLSI design communications networks and management science An international team of 30 40 experts in the field form the editorial board The Handbook of Combinatorial Optimization second edition is addressed to all scientists who use combinatorial optimization methods to

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*Iterative Methods in Combinatorial Optimization* Lap Chi Lau,R. Ravi,Mohit Singh,2011-04-18 With the advent of approximation algorithms for NP hard combinatorial optimization problems several techniques from exact optimization such as the primal dual method have proven their staying power and versatility This book describes a simple and powerful method that is iterative in essence and similarly useful in a variety of settings for exact and approximate optimization The authors highlight the commonality and uses of this method to prove a variety of classical polyhedral results on matchings trees matroids and flows The presentation style is elementary enough to be accessible to anyone with exposure to basic linear algebra and graph theory making the book suitable for introductory courses in combinatorial optimization at the upper undergraduate and beginning graduate levels Discussions of advanced applications illustrate their potential for future application in research in approximation algorithms

Multi-Objective Combinatorial Optimization Problems and Solution Methods Mehdi Toloo,Siamak Talatahari,Iman Rahimi,2022-02-15 Multi Objective Combinatorial Optimization Problems and Solution Methods discusses the results of a recent multi objective combinatorial optimization achievement that considered metaheuristic mathematical programming heuristic hyper heuristic and hybrid approaches In other words the book presents various multi objective combinatorial optimization issues that may benefit from different methods in theory and practice Combinatorial optimization problems appear in a wide range of applications in operations research engineering biological sciences and computer science hence many optimization approaches have been developed that link the discrete universe to the continuous universe through geometric analytic and algebraic techniques This book covers this important topic as computational optimization has become increasingly popular as design optimization and its applications in engineering and industry have become ever more important due to more stringent design requirements in modern engineering practice Presents a collection of the most up to date research providing a complete overview of multi objective combinatorial optimization problems and applications Introduces new approaches to handle different engineering and science problems providing the field with a collection of related research not already covered in the primary literature Demonstrates the efficiency and power of the various algorithms problems and solutions including numerous examples that illustrate concepts and algorithms

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