

# An Improved Chemical Reaction Optimization Algorithm Based on Ant Colony Algorithm

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With the rapid development of computer technology, more and more research organizations and enterprises have turned their attentions from artificial intelligence algorithm to multi-task scheduling. In the face of complex data calculation and task management, natural computing has gradually shown its superiority. As a new method of natural computation, the chemical reaction optimization algorithm has become a new branch of natural computing. In this paper, an improved chemical reaction optimization algorithm is proposed by introducing the ant colony algorithm, which can effectively improve the accuracy and convergence of the chemical reaction optimization algorithm. Firstly, this paper introduces the classification and implementation of chemical reaction optimization algorithm. Secondly, the ant colony algorithm is introduced into the chemical reaction optimization algorithm by introducing the information conversion factor. Finally, ten TSPLIB cases are used as the test object in order to compare with other algorithms. The experimental results show that the improved chemical reaction optimization algorithm based on ant colony algorithm has higher accuracy and efficiency.

## 1. Introduction

Instructions:

In academic research and modern engineering technology, many complex mathematical problems are encountered, which involves a lot of computational problems. So, it is necessary to study the problem of getting optimal solution by computer. With the development of computer technology and artificial intelligence technology, natural computing has gradually become an important field in computational science. Meanwhile, more and more new natural computing methods are proposed.

Natural computing can be seen as a revolutionary calculation after the traditional artificial intelligence, which has a very broad application prospects (Rabinovich, 2003). Natural computing will promote the fundamental development of the systematic, which includes the generalization of the system structure and the expansion of the system field. Nigel (2004) points out that the difference between natural computing and traditional computing system lies in the performance of self-organization, and he discussed the realization of the system from the network and molecular level. Francescoi (2009) reviews the complex data analysis problems in bioinformatics, such as protein structure prediction, microarray data analysis and gene regulatory networks. Wang Peng (2010) analyses the inherent relationship between parallelism and uncertainty in natural computing model, and presents an intelligent model of uncertainty in natural computation. In addition, a large number of computational models based on natural phenomena are proposed. The idea of ant colony optimization is based on the behavior of ant population in path selection and information transfer (Dorigo, 1996). Genetic algorithm is a method to simulate the evolution of biological population by genetic and natural selection (Holland, 1975). Artificial neural network (ANN) is a mathematical model for distributed parallel information processing by referring to the behavior characteristics of animal neural network (Xing, 2013). The optimization algorithm of chemical reaction is an optimization algorithm based on the phenomenon that the molecule is always stable in the low potential energy state. Chemical reaction optimization algorithm plays an important role in industrial production because of its advantages of multi task scheduling.

In this paper, an improved chemical reaction optimization algorithm based on ant colony algorithm is proposed, which can effectively improve the accuracy and convergence of the chemical reaction optimization

algorithm. Firstly, this paper introduces the classification and implementation of chemical reaction optimization algorithm. Secondly, the ant colony algorithm is introduced into the chemical reaction optimization algorithm by introducing an information conversion factor. Finally, ten TSPLIB cases are used as the test object in order to compare with other algorithms. The experimental results show that the improved chemical reaction optimization algorithm has higher accuracy and efficiency.

## 2. Basic theory and method

### 2.1 Chemical reaction optimization algorithm

Chemical reaction optimization (CRO) algorithm is a natural algorithm proposed by Albert and Victor (2010) in Hong Kong. It is a swarm intelligence algorithm based on molecular collision and energy conversion in chemical reaction process. It follows the criterion that each reaction system will respond to its lowest energy state. Through this algorithm, we can solve the problem of finding the optimal solution, so as to solve the calculation problem in many large projects (Li, 2014).

Chemical reaction follows the law of energy conservation. That is to say, the total energy of the whole chemical reaction system is constant.

$$\sum_{i \in A} (EK_{m_i} + EP_{m_i}) + E_{buffer} = K \quad (1)$$

In the above formula,  $EK_{m_i}$  and  $EP_{m_i}$  respectively represent kinetic energy and potential energy of a molecular.  $K$  represents the molecular assembly of the whole chemical reaction system and  $E_{buffer}$  represents central energy buffer.  $K$  is a constant which represents the total energy of the whole chemical reaction system.

At the same time, the chemical reaction can meet the following conditions.

$$\sum_{i=1}^A (EK_{m_i} + EP_{m_i}) \geq \sum_{i=1}^B EP_{m'_i} \quad (2)$$

According to the changes of molecular structure and the number of molecules involved in the reaction, it can be divided into monomolecular reaction and multi molecular reaction. The monomolecular reaction includes molecular decomposition and the collision between molecule and the system boundary. Multi-molecular reaction includes molecular synthesis and intermolecular collision.

#### (1) Collision between molecules and system boundary

This kind of collision refers to the process of obtaining a neighbouring molecule after the collision between molecules and the boundary of the system. We assume that the molecular structure before collision is  $m$ , and the molecular structure after collision is  $m' = N(m)$ . According to the law of conservation of energy, we can get the formula.

$$EK_m + EP_m \geq EP_{m'} \quad (3)$$

The kinetic energy after molecular collision can be get by the following formula.

$$EK_{m'} = (EP_m + EK_m - EP_{m'}) \cdot \sigma \quad (4)$$

where,  $\sigma$  means the loss rate of kinetic energy, and it satisfies the condition  $\sigma \in (0, 1]$ .

#### (2) Molecular decomposition

Molecular decomposition is the process that one molecule is broken down into multiple molecules after the collision with the system boundary. We assume that the molecular structure before collision is  $m$ , and the molecular structure after collision are  $m'_1, \dots, m'_n$ . The whole reaction process meets the following conditions.

$$EK_m + EP_m \geq \sum_{i=1}^n EP_{m'_i} \quad (5)$$

Since the central energy buffer can complement the potential energy of the decomposed molecules, the conservation equation when the central energy buffer is considered can be get as follows.

$$EK_m + EP_m \geq \sum_{i=1}^n EP_{m'_i} \quad (5)$$

$$EK_m + EP_m + E_{buffer} \cdot \prod_{i=1}^n \sigma_i \geq \sum_{i=1}^n EP_{m'_i} \quad (6)$$

where, the parameters are independent of each other, and it meet the condition  $\sigma \in (0,1]$ .

### (3) Intermolecular collision

The intermolecular collision is the process that some molecules collide with each other and produce the same number of new molecules. We use  $m_1, m_2$  to represent the molecular structure before collision, and use  $m_1', m_2'$  to represent the molecular structure after collision. The intermolecular collision follows the following conditions.

$$EK_{m_1} + EP_{m_1} + EK_{m_2} + EP_{m_2} \geq EP_{m_1'} + EP_{m_2'} \quad (7)$$

Then, we can get the kinetic energy of the new molecule after collision.

$$EK_{m_1'} = [(EK_{m_1} + EP_{m_1} + EK_{m_2} + EP_{m_2}) - (EP_{m_1'} + EP_{m_2'})] \cdot \sigma \quad (8)$$

$$EK_{m_2'} = [(EK_{m_1} + EP_{m_1} + EK_{m_2} + EP_{m_2}) - (EP_{m_1'} + EP_{m_2'})] \cdot (1 - \sigma) \quad (9)$$

### (4) Molecular synthesis

Molecular synthesis refers to the process that many molecules collide with each other and fuse into a new molecule. We let  $m'$  as the new molecule after collision, and the reaction process satisfies the following formula.

$$EK_{m_1} + EP_{m_1} + EK_{m_2} + EP_{m_2} \geq EP_{m'} \quad (10)$$

## 2.2 The realization of CRO

Table 1: The parameter and meaning

Parameter	Meaning
$T$	Molecular aggregation
$R_{loss}$	Loss rate of kinetic energy
$D_e$	Determining factor of Molecular reaction
$EK_{initial}$	Initial kinetic energy
$E_{buffer}$	Central energy buffer
$\gamma$	The control factor of single molecule
$\mu$	The control factor of Multi-molecule

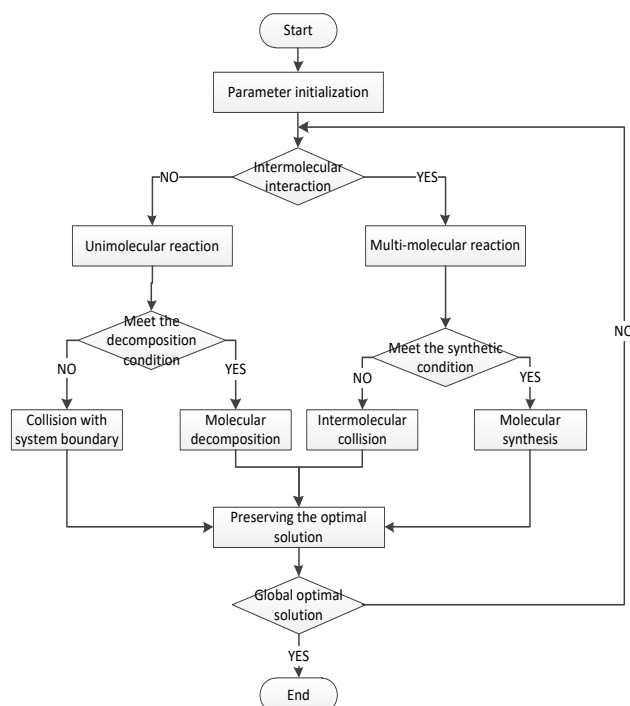


Figure 1: The flow chart of CRO

Generally speaking, the whole process of chemical reaction optimization algorithm can be divided into three parts, and they are respectively the initialization of molecular structure, molecular collision and validation of collision result. The flow chart of CRO is as follows.

#### Initialization of system parameters

The parameters of the chemical reaction system are set according to the practical problems. And the main parameters in the algorithm initialization are shown in the following table.

#### Check the type of molecular collision

Take a random number  $\theta(\theta \in (0, 1])$ , if  $\theta < D_e$ , the system will carry on the multi molecular collision. Otherwise, it will carry on single molecule collision.

#### Monomolecular collision

When the times optimal solution appeared reaches  $\gamma$ , the molecules in the system will be broken down into several new molecules. Otherwise, there will be an invalid collision between molecular and system boundaries.

$$Hit_{num} - Hit_{min} > \gamma \quad (11)$$

#### Multi molecular collision

If the kinetic energy of the selected molecules is less than  $\mu$ , it will carry out the synthesis of molecules. Otherwise, there will be no effective collision between molecules

$$EK < \mu \quad (12)$$

#### (5) Validation of collision result

At the end of the molecular collision, we can judge whether the reaction has a lower objective function value. If so, the optimal solution of the reaction is recorded. If not, there will be a new round of molecular collision.

### 3. Improved chemical reaction optimization algorithm

Because of the slow convergence speed and low precision of the chemical reaction optimization algorithm, we try to introduce the ant colony algorithm into CRO based on its fast convergence speed. By establishing the transformation strategy, we successfully achieve the convergence of the two algorithms.

We define that the initial pheromone of ant colony algorithm is  $\varphi$ , which consists of two parts.

$$\varphi = \varphi_c + \varphi_{CTA} \quad (13)$$

In the formula,  $\varphi_c$  is the pheromone constant, which is usually set in the initialization phase according to the specific situation.  $\varphi_{CTA}$  is the value of the conversion strategy proposed in this paper, which is used to realize the convergence between CRO and ACO.

Because of the uncertainty of the molecular set in the CRO algorithm, the number of the optimal solutions we get is also uncertain. So, it is necessary to adjust the size according to the fitness value. Assuming that the number of elements in the optimal solution set is  $v$ , when the number of optimal solutions obtained by CRO is less than  $v$ , we will randomly extract several second-best solutions to make the number of population equal to  $v$ . Similarly, if the number of optimal solutions obtained by CRO which is more than  $v$ , we will remove some solutions according to the fitness value in order to make the population number equal to  $M$ .

$$Num_{sub} = \begin{cases} v & Num_{pop} \geq v \\ v & Num_{pop} < v \end{cases} \quad (14)$$

Then, the intensity of the pheromone between  $i$  and  $j$  can be get.

$$\varphi_{ij} = \frac{k_{ij}}{v} \quad (15)$$

where,  $k_{ij}$  is the number of paths between city  $i$  and  $j$ .

$$\varphi_{CTA} = \begin{pmatrix} \varphi_{11} & \cdots & \varphi_{1j} & \cdots & \varphi_{1n} \\ \vdots & & & & \vdots \\ \varphi_{i1} & & \ddots & & \varphi_{in} \\ \vdots & & & & \vdots \\ \varphi_{n1} & \cdots & \varphi_{nj} & \cdots & \varphi_{nn} \end{pmatrix} \quad (16)$$

The steps of the improved chemical reaction optimization algorithm are as follows.

#### The initialization of system

The system randomly generates n molecules in order to form an initial set, where, the setting of variable n is related to the scale of specific problems.

#### Setting the fitness function

Because in the ant colony algorithm, each ant can't go through a city more than one time, the fitness value can be set as follows.

$$K_{\min} = \sum_{j \in \text{City}} \sum_{i \in \text{City}} u_{ij} \cdot v_{ij} \quad (17)$$

#### Obtaining the optimal solution by CRO

The optimal solution is obtained by chemical reaction optimization algorithm

#### Convergence of ant colony algorithm

The optimal solution is transformed into the initial pheromone of ant colony algorithm by pheromone conversion strategy proposed above.

#### Getting the optimal solution

The initial pheromone is applied to the ant colony algorithm, and the optimal solution can be get at last.

## 4. Simulation experiment and result analysis

In order to verify the effectiveness of the improved chemical reaction optimization algorithm, this paper selects 10 examples in TSPLIB to carry out simulation. In the simulation experiment, we set  $R_{\text{loss}}=0.73$ ,  $D_e=0.25$ ,  $EK_{\text{initial}}=1200$ ,  $v=60$ ,  $\gamma=4$ .

Table 2: The parameter and meaning

Algorithm	ACO		CRO		SA		ICRO	
TSPLIB	optimum solution	Error	optimum solution	Error	optimum solution	Error	optimum solution	Error
RAT99	2489	0.37	2489	0.37	2490	0.38	2488	0.35
LIN318	6133	0.3	6136	0.31	6135	0.29	6124	0.28
BAYG29	2390	0.23	2391	0.26	2388	0.22	2385	0.21
PR439	11913	0.41	11915	0.43	11917	0.44	11908	0.4
FL417	21499	0.38	21496	0.35	21492	0.34	21490	0.31
EI151	127005	0.26	127070	0.29	127112	0.31	126958	0.25
SIL75	42216	0.33	42252	0.26	42237	0.24	42216	0.33
CH130	21329	0.23	21337	0.26	21328	0.22	21329	0.23
HK48	1610	0	1617	0.03	1610	0	1610	0
GR17	439	0.32	435	0.30	427	0.27	426	0.25

At the same time, in order to directly evaluate the improved algorithm, we use also use the basic chemical reaction optimization algorithm (CRO), ant colony optimization algorithm (ACO), simulated annealing algorithm (SA) to simulate under the same conditions and finally get the results as follows.

$$\mu = \frac{\sum_{i \in T} EP_i}{2} \quad (18)$$

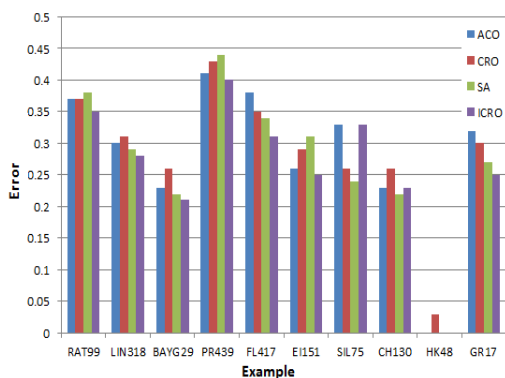


Figure 2: The relationship between experimental cases and error

The relationship between experimental cases and accuracy in the simulation experiment is shown in figure 2. Through the experimental analysis, we can get that the improved algorithm has some improvement in accuracy compared with ACO, CRO and SA. However, because of the complexity of the new algorithm, the computational time is a little longer than the traditional chemical reaction optimization algorithm, which affects the application of the algorithm to some extent.

## 5. Conclusion

The combination of different algorithms is a simple and effective strategy to improve the performance of the algorithm. Compared with the traditional chemical reaction optimization algorithm, the improved algorithm has the advantages of convergence and accuracy, which plays an important role in multi task scheduling. We hope that the research in this paper can promote the development of natural algorithm theory to some extent, especially in the field of intelligent design.

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