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Ant Colony Optimization: A Leading Algorithm in Future Optimization of Chemical Processes

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Abstract

Ant colony optimization is a metaheuristic algorithm whose power leads to lower computational cost to optimize complicated problems. Although usually used for discrete domains, this algorithm with some necessary modifications has been applied to continuous optimization. Two examples with varying degrees of complexities are presented as an illustration for solving a large class of process optimization problem in chemical engineering. This algorithm is simple to implement and the results of case studies shows its ability to provide fast and accurate solutions.

Keywords

Ant Colony, Optimization, Process, Methanol Reactor

1. Introduction

Ant colony optimization (ACO) was introduced as a novel nature-inspired metaheuristic by M. Dorigo et al. [1]. A metaheuristic refers to a master strategy that guides and modifies other heuristics to produce solutions beyond those that are normally generated in a quest for local optimality. ACO is mainly applicable to discrete optimization problems such as the traveling salesman problem [2]. However, it can be also applied to continuous domains such as optimal design and scheduling of batch plants [3], optimization of liquid-liquid

extraction process [4]. In the present study, a new version of multi-dimensional ACO for continuous domain has been introduced by combining ACO with a direct-search method. Two examples with varying degrees of complexities were presented as an illustration for solving a large class of process optimization problems in chemical engineering.

2. An Overview of ACO

Ant colonies are distributed systems that in spite of the simplicity of their individuals, presents a highly structured social organization. As a result, it makes it possible to do hard tasks [1]. The main idea of this method is derived from the real ant foraging behavior. Ants search randomly to find food. As soon as they find food, in the way back, they produce chemicals that are called pheromones. By producing pheromone, each ant helps others to pursue the marked way indirectly and find food faster. Although amount of pheromone will decrease due to vaporization, but this also helps colony to explore new ways instead of only one way. When amount of pheromone is increased in one way, other ants find this way more attractive and follow the same way.

2.1. ACO Algorithm for Continuous Domain

In order to apply ACO algorithm in continuous domain a new data structure is needed. The data structure which has been used in this work is shown in Fig. 1. The two dimensional $n \times m$ matrixes is the search area where n is the number of variable to be optimized and m is the number of ants (i.e., regions in continuous domain) which are used to search with $m \geq n$ [1]. f_i and τ_i are $1 \times m$ vectors representing the ith region objective function and pheromone trail amount, respectively.

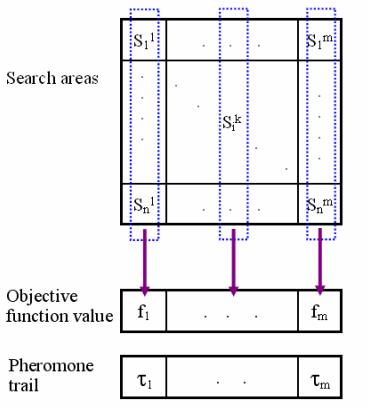

Fig. 1 CACO data structure

2.2. Continuous Ant Colony Optimization (CACO) Algorithm

The CACO algorithm is described below.

a) Initialization
In this stage each region is randomly initialized for each variable in the feasible interval. Feasible interval is defined by problem constraint. The equal amount of pheromone is also placed in pheromone trail vector.
b) Global search

The main responsibility of global ants is to search globally in order to escape local optimum traps. The global search consists of three operations: crossover, mutation and trail diffusion. In mutation, each ant jumps into a new region according to Eq. (1). Trail diffusion is a stage in which two parent ants are randomly chosen and the new infant is born to keep the behavior of parents.

$$\text{step for variable i} = (-1)^{1+\text{rand}(1)} \times \max.\ \text{step for i} \times (1 - r^{(1-t/t_{max})^{b}}) \qquad (1)$$

The new coefficient $(-1)^{1+\text{rand }(1)}$ is added to the main equation in this work to make the direction of jump randomly in both direction.

c) Local search

Local ants search in a smaller region around the potential solution to improve the objective function. Different methods such as simulated annealing could be used for local search [5]. Direct search is used in the present work to decrease the load of computation in this stage. Direct search checks nearby regions in both directions of each variable to find a better solution.

d) Pheromone update

Trail evaporation is used in order to ensure that the search during the next generation is not biased by the proceeding iteration. The pheromone trail is updated after each iteration as follows:

$$\tau_i^{(t+1)} = \begin{cases} (1-\rho)\,\tau_i^{(t)} + dr_i^g & \text{fitness improved} \\ (1-\rho)\,\tau_i^{(t)} & \text{otherwise} \end{cases} \qquad (2)$$

This new definition for adding pheromone used in this work was found to be better than the one used before [3] which is based on the fitness improvement. In the new pheromone update strategy, Eq. (2), evaporation and laying pheromone is kept in the proportional range and would prevent stagnation in the local minima.

3. Problem Definition

Lurgi's methanol technology uses a dual reactor system for synthesis of methanol (Fig. 2) [6]. The methanol synthesis reactions rates on commercial $Cu/Zno/Al_2o_3$ can be found on [7]. In the present study, the reactors are modeled base on a homogeneous one- dimensional fixed catalytic bed model in steady state .The mass and energy balances are shown as follows:

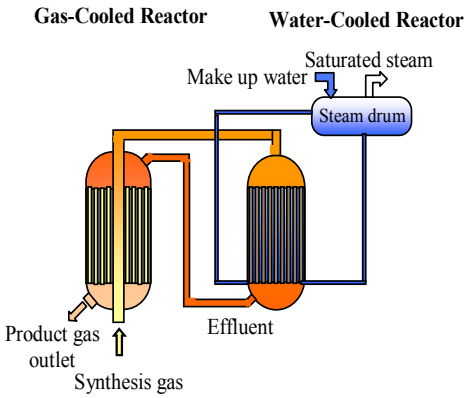

Fig. 2 Methanol Reactors of Lurgi's Process

$$\frac{dX_{i,k}}{dz} = A_k R_i (X_{1,k}, X_{2,k}, T_k) \tag{3}$$

$$\frac{dT_k}{dz} = \frac{1}{GC_p}\left[\frac{4U}{d}(T_{wall} - T) + \left(-\sum_i \Delta H_i R_i (X_{1,k}, X_{2,k}, T_k)\right)\right] \tag{4}$$

$$X_i = \frac{F_j - F^o_j}{\alpha^i_j} \qquad F_{TOT} = F^o_{TOT} + \sum_{i,j} \alpha^i_j X_i \tag{5,6}$$

In the present study, the objective is to reach the maximum methanol production yield in the effluent of the gas cooled reactor.

$$\begin{aligned} \text{Max} \quad & y_{MeOH} F_{TOT} \\ \text{s.t.} \quad & 230\ ^{O}C \le T_{shell} \\ & 0 \le y_{CO}, y_{CO_2}, y_{H_2} \le 1 \end{aligned} \tag{7}$$

Two cases were considered for optimization:
Case 1: The control variable is the temperature of the steam drum, i.e., shell temperature of the water cooled reactor. This is a single variable optimization problem.
Case 2: The control variables are feed composition of the system. This is a multi variable optimization problem.

4. Results and Discussion

The two cases were solved using the CACO parameters shown in Table 1. In case 1 (single variable) CACO converges to the solution after only 6 iterations. The optimum value of shell temperature that increase the amount of methanol by 3.17 % is 233.9 ^{0}C. The result of the feed composition optimization is shown in Table 2 and the amount of methanol production increase by 2.54 %.

Table 1. Ant colony parameters

	Ants	Crossover Probability	Mutation Probability	Evaporation rate	Local ants %
Case 1	20	50	40	0.9	40
Case 2	20	60	50	0.95	45

Table 2. Methanol reactors feed composition (mol fraction %)

y_{CO}	y_{CO2}	y_{H2}
5.72	12.64	63.41

Figures 3 and 4 illustrate the performance of the modified CACO algorithm for case 1. The performance of the old strategy [3] is also shown in these figures. Figure 3 corresponds to the modification done in global search strategy (Eq. 1) and Figure 4 corresponds to the modification done in pheromone update (eq. 2). It could be seen in both figures that convergence (i.e., mean population should be close to best) in the modified algorithm is considerably faster than the old algorithm.

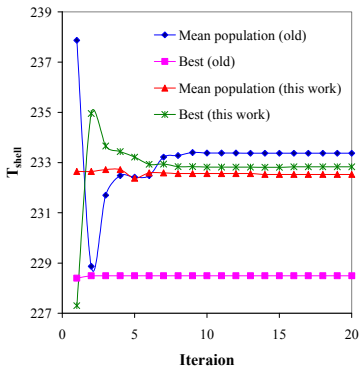

Fig. 3. Effect of modification in local search strategy on CACO convergence.

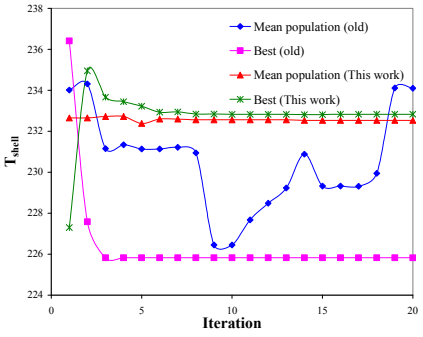

Fig. 4. Effect of modification in pheromone update strategy on CACO convergence.

5. Conclusions

In the present study, an improved ACO data structure and algorithm for multi dimensional optimization has been developed. The algorithm is simple and fast compared to the conventional algorithm and could be applied to problems with different degree of complexity. This algorithm was successfully applied to the problem of methanol synthesis for both single and multiple dimensions. The ant colony approach could be included in the list of future reliable and useful optimization tools in chemical engineering.

Nomenclature

A	Reactor transversal area (cm^2)
C_p	Mean specific heat (cal/g/K)
d	Reactor diameter (cm)
F	Molar flux (mol/s)
G	Mass flux ($g/cm^2/s$)
R	Reaction Rate ($mol/s/cm^2$)
T	Temperature (K)
T_{wall}	Reactors wall temperature (K)
U	Overall heat transfer coefficient ($cal/s/cm^2/K$)
X	Extent of reaction (mol/s)
z	Reactor axial variable
α	Stoichiometric coefficient
ΔH	Enthalpy (cal/mol)
TOT	Total
i	Number of independent reactions
j	Key components (CO, MeOH)
k	Reactor index

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