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# Dynamic Multi-objective Optimization of Chemical Process Based on Bare Bones Particle Swarm Optimization

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The purpose of this study is to improve the production efficiency and safety of chemical process. To this end, the dynamic multi-objective optimization of chemical process based on bare bones particle swarm optimization (BBPSO) was studied in this paper. Firstly, the algorithm of BBPSO was studied. On this basis, the algorithm was improved in terms of its search performance. Then, the constraint treatment method was designed and used for simulation experiments. Experimental results show that to produce the 6.125g of foreign protein, it only needs to add the 439ML inducer. Therefore, the proposed algorithm exhibits better convergence and distribution, achieving the optimization effect.

## 1. Introduction

The quality of chemical products is closely related to the chemical production process. Advanced chemical processes can reduce impurities and further improve the quality of products. At this stage, the production technology and process of China's chemical enterprises varies from each other, and the quality of the products developed is also quite different. However, for some chemical enterprises, their chemical technologies and processes are relatively backward, and the equipment is outdated, seriously polluting the environment and making it difficult to ensure the current chemical safety. Based on this, this paper first studies the BBPSO algorithm, and then improves the algorithm in terms of its search performance. After that, the dual-segment mechanism constraint treatment method was designed and used for simulation experiments.

## 2. Literature review

The particle swarm optimization algorithm has the advantages of simple optimization principle, less adjustable parameters, parallel search and global convergence. It has proven to be effective in practical applications. The algorithm is based on the behavior of birds flying in the natural world for foraging. At present, there is no complete proof for the convergence of particle swarm optimization. Many scholars have carried out a convergence analysis based on the topological structure of particle swarm particle motion trajectory for this problem, and given the corresponding theorem to guarantee the global convergence of the algorithm. In addition, in the theoretical study of particle swarm optimization algorithm, the update mechanism of particle velocity and position is studied. A new way of updating is proposed (Chen et al., 2014). The algorithm is updated only if there is no obvious change in fitness value, which helps the algorithm to jump out of local convergence. However, this improvement may lead to a decrease in the convergence speed of the algorithm (Fan et al., 2017). A law indicating the relationship between the psychological quantity and the physical quantity is added to the update formula of speed and position, so that the particle can perform optimization more effectively. At the same time, the particle topology of the particle swarm optimization algorithm has also been studied accordingly. The modification of the topology structure can help the particles to better optimize during the flight process. The trajectories of particles are studied, and the influence of particles on the inertia terms in particle swarms is empirically analyzed. Finally, a multi-dimensional stochastic particle swarm optimization algorithm is proposed. The particle swarm optimization algorithm has a simple optimization principle and few calculation parameters. How to choose different parameter values has a significant impact on the performance of the algorithm. In general, the study of modified parameters for particle swarm

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optimization is mainly for the following parameters: inertia weight and learning factor. By studying the dynamic modification or static assignment of these parameters, the optimization efficiency of the particle swarm optimization algorithm and the ability to jump out of the local optimum can be effectively improved.

By modifying the value of the inertia weight in the particle swarm algorithm update formula, the ability of the algorithm to explore the unknown solution space and the ability to approach the optimal solution can be controlled. When the decreasing inertia weight value is used, the initial inertia weight is larger, and the algorithm tends to search globally. The ability of particles to explore the unknown solution space is strong. As the algorithm continues to move, the inertia weight value decreases, and the algorithm tends to local search. The ability of particles to approach the optimal solution is gradually enhanced. The inertia weight is taken as a random number uniformly distributed in the interval [0, 1]. A new adaptive inertia weighting method is proposed (Feng et al., 2015). The success rate of the particle group is used as a feedback parameter to determine the particle's position in the search space. An improved particle swarm optimization algorithm is proposed to improve the performance of the standard particle swarm optimization algorithm. The dynamic inertia weight of the algorithm increases with the number of iterations (Han et al., 2017). The learning factor is also a key research branch of the particle swarm algorithm. Usually, these two learning factor values are often set to 2.0. At the same time, the particle swarm optimization algorithm may have some drawbacks in the actual optimization application process. For example, the algorithm is premature, the convergence speed is slower, and the optimization result of the algorithm is not high. In order to overcome the premature phenomenon of particle swarm optimization, many scholars combine particle swarm optimization with other algorithms with excellent convergence properties. The particle swarm algorithm is combined with the difference algorithm, which can effectively avoid the premature phenomenon caused by the particle swarm algorithm and improve the search ability and efficiency. A particle swarm optimization algorithm based on the combination of evolutionary thinking and Gaussian variation is proposed. The algorithm combines traditional speed and position update rules with the idea of Gaussian variation. The particle swarm algorithm and the simulated annealing algorithm are combined. By simulating the global optimization performance of the annealing algorithm, the premature problem of the particle swarm algorithm is solved. A hybrid particle swarm optimization algorithm is proposed. On the one hand, combined with the difference algorithm, the algorithm helps the particle swarm algorithm to globally converge; on the other hand, combined with the penalty function method, the constrained optimization problem is solved. Aiming at the problem of optimal scheduling, a particle swarm optimization algorithm based on fuzzy selection and differential algorithm is proposed. In addition, the particle swarm algorithm is simple to set up with few parameters and is easy to combine with other algorithms (Rangaiah et al., 2015). Therefore, many discussions have evolved into research: how to combine particle swarm optimization algorithms with other engineering-specific algorithms in a scientific and rational way to improve the optimization efficiency process.

An important criterion for evaluating the value of optimization theory and algorithms is to guide practical applications and better serve practical applications. Due to the advantages of simple particle swarm optimization, less optimization parameters and fast convergence, the algorithm is widely used to solve various engineering practical problems. Single-objective optimization and multi-objective optimization problems are first distinguished based on specific issues. At the same time, it is also classified according to the nature of the design parameters. Generally, it can be divided into two types of problems: continuous parameter optimization and discrete parameter optimization. At present, the research of PSO algorithm is mainly aimed at solving the continuous parameter optimization problem. From the pixels sampled by the image, the weight of the color discrimination transformation matrix is solved. The particle swarm algorithm is used to obtain the fitness value of the k-center point. Compared to some mathematical optimization algorithms, such an optimization method can quickly and easily implement fire system detection. A new hybrid algorithm was proposed to determine the development of the most relevant genes involved in breast cancer. Combined with the teaching and learning optimization algorithm and the proposed mutation fuzzy adaptive particle swarm optimization algorithm, the minimal subset of genes involved in breast cancer was found. The results show that the proposed technique can achieve an accuracy of 91.88%. An improved PSO algorithm for parameter identification of nonlinear dynamic hysteresis models is proposed. Studies have shown that this improvement reduces the impact of randomness using particle swarm optimization (Roy and Bhui, 2016).

The discrete particle swarm optimization algorithm is mainly for solving the combinatorial optimization problem. At present, researchers are also working to improve the application of particle swarm optimization in discrete parameters. A binary discrete particle swarm optimization algorithm is proposed. The algorithm represents the position of the particle as 0 or 1, and the velocity of the particle is represented by the value between 0 and 1. Through such a binary representation method, the algorithm can be optimized in discrete space. In solving the vehicle routing problem, the position and velocity update formula of the original continuous particle swarm optimization algorithm is used. However, after the position and velocity information is rounded, the corresponding discrete optimization results can be obtained. A new discrete particle swarm optimization algorithm based on quantum individual is proposed. It is simpler than existing algorithms, and its simulation experiments and its application in code division multiple access also prove its high efficiency. A new discrete particle swarm optimization algorithm design idea is proposed, and the improved algorithm is applied to travel business travel problems. A new binary particle swarm optimization method based on immune theory is proposed (Vallerio et al., 2016). The simulation results show that the proposed algorithm has improved search ability and convergence speed compared with other binary particle swarm optimization algorithms and genetic algorithms.

All the above studies were conducted on single-objective optimization problems. However, in the actual application of engineering, there is more than one goal for optimization. Variables are often associated, non-independent, and even present a contradictory trend. Therefore, the particle swarm optimization algorithm for multi-objective optimization problems is gradually being included in the research object. In the standard particle swarm algorithm, the Pareto dominance concept and the mechanism of the optimal solution found in archive storage are introduced, and a multi-objective particle swarm optimization algorithm is proposed. The algorithm can select the global optimal solution through the above two selection mechanisms and obtain a series of non-dominated solutions (Zhang et al., 2015). This algorithm is also one of the most commonly used methods for dealing with multi-objective problems. In 2002, the first multi-objective particle swarm algorithm using the archiving mechanism was proposed. On this basis, in order to increase the convergence ability of CMOPSO algorithm, a hybrid multi-objective particle swarm optimization algorithm is proposed. The theoretical research on particle swarm optimization is mainly focused on the single-objective particle swarm optimization algorithm. The corresponding theoretical research results of the multi-objective particle swarm optimization algorithm are few. Corresponding analysis is made on factors that affect one or more aspects of the performance of the algorithm. In applied research, in 2013, the application of multi-target particle swarms was reviewed in detail. The application areas are divided into sixteen categories: urban planning, data mining, industrial engineering problems, workflow optimization, image processing, aerospace engineering, robot path optimization, software engineering, and neural network training.

To sum up, at present, most of these algorithms focus on unconstrained problems. There are few studies on constrained multi-objective optimization problems. Chemical processes often need to set corresponding constraints to meet certain safety operations and product performance indicators. Constraint processing is one of the key parts. It is necessary to establish an effective method to solve the general constrained multi-objective optimization problem. Moreover, most of these algorithms focus on how to get the optimal solution or approximate optimal solution that satisfies the condition as much as possible, and the effectiveness of the algorithm and the quality of the solution are rarely considered. Therefore, for the multi-objective dynamic optimization problem of constrained chemical processes, in order to achieve better processing of constraints and improve the search ability of the algorithm, a new hybrid constraint processing method is adopted. The dynamic multi-objective optimization of chemical process is studied by the backbone particle swarm optimization algorithm.

## 3. Principles and methods

The numerical method is used to discretize the optimization problem of infinite dimension, and the optimal drawing trajectory is approximated by the discrete curve line, which is then transformed into Euclidean optimization problem. That is, the time interval of the dynamic system is discretized, and the optimal control trajectory for each time interval is obtained to convert the dynamic into the static optimization problem.

Sierra and Colleo have comprehensively summarized the current multi-objective particle swarm optimization algorithm, which is categorized into: aggregation method, dictionary order method, sub-population method, Pareto-based method, ε-dominant method, hybrid method, and other multi-objective particle swarm optimization algorithms. Although the speed update formula of the standard PSO algorithm is a random form, the results are not random, since the particles are not independent, e.g., it is also affected by the speed direction of the previous generation, which may cause the particles to stay longer on the same side of the previous optimal particles. In contrast, the structure of the Gaussian distribution method is more advantageous in certain degree. A large number of experimental studies have shown that BBPSO's probability search method is simple and easy to implement, with no need to repeatedly adjust the appropriate parameter values like the traditional particle swarm algorithm, and it can also significantly improve the efficiency and accuracy of the algorithm search. So, BBPSO is a type of PSO algorithm with better performance. The dynamic multi-objective dynamic problem model of chemical process is often complicated. Thus, the algorithm needs to be fast in convergence and computationally inefficient, so as to obtain a high-quality optimal solution with wide distribution and uniform convergence performance.

In the standard PSO algorithm, the inertia weight is used to control the influence of the historical speed of the particle on the current speed; the acceleration factor is used to balance the individual and group cognitive ability, which has an important impact on the convergence performance. In order to better balance the global search and local development capabilities of the algorithm, the inertia weight and acceleration factor in the particle update equation change dynamically with the iteration. In the later stage, most of the optimal particles are close to or have been at the front of Pareto, and the particles are more locally optimized near the global optimal particles. Meanwhile, as r2 decreases, the step size for optimization is reduced, to improve local optimization ability. In Figure 1, points A and B respectively represent the global and local optimal points when searching for a certain number of algebras. According to formula 6, for the particles, the intermediate point C is taken as mean value, and the XA-XB as the standard deviation for the Gaussian distribution.Figure2 shows the probability of value. After making improvement, in the initial stage of the search, the greater probability of the particle group can be searched near F which is not the global optimal points, thereby improving the global search ability.


*Figure 1: Illustration of position updating*

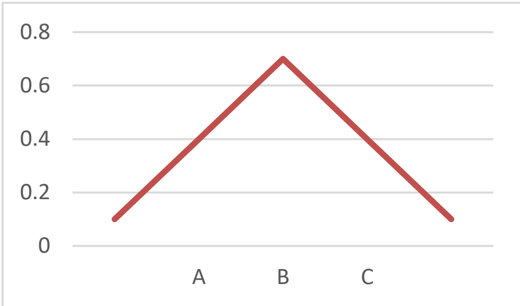



*Figure 2: Illustration of probability distribution*

In this paper, a combination method of the multi-objective particle swarm optimization algorithm and the control vector parameterization method was applied to the dynamic multi-objective optimization problems. The simple control parameterization method is as follows: first, divide the time interval into D equal parts, ... < tD, <tD < tf, and each time interval length l = (tf - t0)/D; then, the control variables are represented on each interval by some constant functions, linear functions, polynomial functions, and B-spline functions, etc., so that the control variables are denoted by the piecewise functions of some parameters, and the dynamic optimization problem is transformed into the parameter optimization problem.

In this paper, the control variable U is expressed as a constant value in each time interval, and the control parameter U= [ui, U2, ... UD] represents a solution to the original problem. The BBPSO algorithm is applied in each time period to solve the multi-objective optimization problem. The initial population of U is firstly generated by MOPSO; for each U, it represents the change trajectory of each control variable u(t), and the Rune-Kutta method is used to solve the system of ordinary differential equations in each time interval. After iterations for D times, each state variable x(t) is obtained., and then each objective function value is calculated; next, the BBPSO is used to perform position update operation, and evolve into new population; It's detected whether the termination condition is satisfied; if not, repeat the first few steps; finally, the optimal solution set is output. Figure2 shows its flow chart. The number of segmentation is greatly related to the optimization results. In general, the more segments, the more dimensions of the optimization problem, the more iterations are performed, and the better the optimization effect, but with more computations.

In this paper, the modified bare bones particle multi-objective swarm optimization algorithm is abbreviated as NBBMOPSO for the solving dynamic optimization problems. For comparison, a multi-objective particle swarm optimization algorithm (H_MOPSO) and an unmodified bare bones multi-objective particle swarm optimization algorithm (BBMOPSO) were also used to solve dynamic multi-objective models of several chemical production processes. The maximum number of iterations for several algorithms was set to 300 generations, and the external file set capacity was 200. All other parameters were consistent. For the improved algorithm, in the parameter setting of the Gaussian mutation, the starting mutation probability is 0.5 and the termination probability is zero. It ran 20 times independently for each case, perform statistics after the test, and then conducts algorithm performance analysis based on the results obtained from the test.

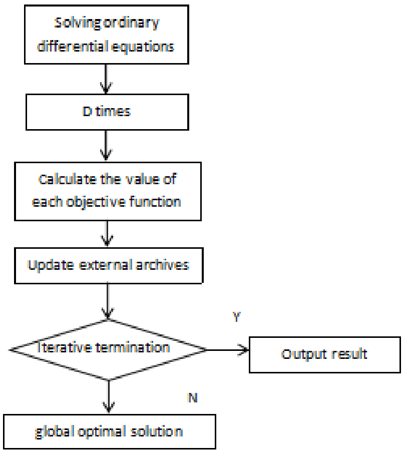
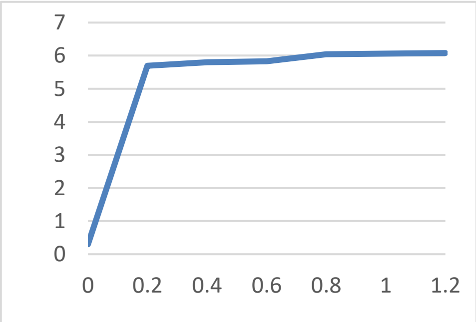



*Figure 3: The flow diagram for the basic frame of DBBMOPSO*

## 3. Results and analysis

For this dynamic multi-objective case, the two control variables were divided into 8 segments empirically; Figure4 is the Pareto non-dominated solution set obtained by BBMOPSO, in which the x-axis indicates the addition amount of the inducer, and Y-axis is the final yield of foreign protein. All points at the Pareto optimal frontier reflect the value of inducer addition and exogenous protein yield under different optimal decisions, which can be used to make analytical decisions.



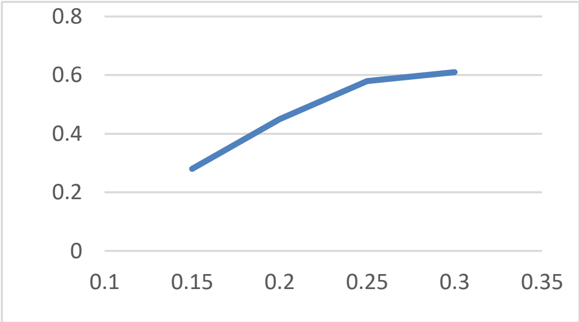




*Figure 4: The Pareto solutions found by MBBMOPSO for easel*

*Figure 5: The Pareto frontier from the algorithm*

From the figure above, the yields of exogenous protein obtained at four points were 2g, 5g, 6g and 6.150g, respectively, while the amount of inducer added were 0.0024L, 0.0189L, 0.0980L and 1.3919L, respectively. It can also be seen that within a certain range, it's very sensitive to addition of the inducer, and the addition of 0.0024L inducer increased the yield from 0.17 g to 2g; whereas, outside one certain range, the total amount of inducer added ranged from 0.0980L to 1.3919L, while the yield of exogenous protein only increased from 6g to 6.150g. When the price of the inducer is not expensive, the maximum economic benefit can be obtained by taking the right adding strategy on the right side, and when it is relatively expensive, it is suitable to adopt the strategy on the left side of the figure.
In this case, the control variables were equally divided into 8 segments, and the other parameters were set as above. Figure5 shows the Pareto frontier obtained by this improved algorithm. The horizontal and vertical coordinates are the concentrations of reactants and intermediates at the end of the reaction. It can be seen from the figure, the concentration of the reactant increased from 0.25 to 0.3, and the concentration of the intermediate product increased from 0.59 to 0.61. Therefore, if the concentration of the lower reactant is the important indicator, it is appropriate to take the temperature control scheme corresponding to the intermediate point.
Table 1 shows the comparison results of the two algorithms. It can be seen from Table 1 that, in terms of convergence, the BBPSO algorithm has better advantages than other PSO algorithms in solving dynamic

multi-objective problems, and the improved BBPSO can obtain more competitive Pareto optimal solution. Moreover, from the extreme value solution, the improved algorithm obtains the optimal solution with wider distribution, so as to better provide decisions. Also, the implementation of the BBPSO is simpler. It does not require a speed position update form, as long as the Gaussian distribution is used. Other standard particle swarms have a greater influence on the optimization, and the optimal value should be adjusted. In this case, the improved BBPSO algorithm showed better performance. For the parameter adjustment, it has a great influence on the optimization result. In the parameter adjustment, the number of segments transformed from dynamic problems has greater impact on optimization results

*Table 1: Comparison of S measure (mean and standard deviation)*

| S | problem 1 | problem 2 |
|---|---|---|
| Backbone particle swarm optimization | 0.0205<br>6.00E-03 | 0.0628<br>2.02E-02 |
| Improved backbone particle swarm optimization | 0.0311<br>5.00E-03 | 0.0964<br>8.60E-03 |

## 5. Conclusions

Experiments on dynamic multi-objective optimization of chemical process show that in addition to the characteristics of PSO algorithms such as fast convergence and simple principle etc., the improved simple bare bones multi-objective particle swarm optimization algorithm proposed in this paper has better global solution performance and a stronger extreme value solving ability. It can ensure to obtain a more highly competitive optimal solution set that is approaching to the real Pareto, and achieve greater advantages than other algorithms when solving the dynamic multi-objective optimization problem. This can provide effective and flexible support for the decision analysis of the practical problem.

In this paper, a dynamic BBPSO algorithm was proposed for the dynamic multi-objective optimization problem of chemical process, which better handles this kind of problem. However, based on the author's limited ability and time constraints, there is still much work to be further studied. When the experiment of actual cases was carried out, it's found that the algorithm has a slower rate in jumping out of the local optimal solution under the condition of more constraints.

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