The use of the harmony search method in chemical kinetics problems: a literature review

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Abstract. This paper considers and reviews the publications about the Harmony search algorithm and applications of the Harmony Search algorithm. It approaches to achieve perfect results in a huge number of optimization problems. The paper analyses the literature on the application of Harmony Search algorithm to supply the future research directions. That Harmony search algorithm will be used to calculate the reaction kinetic parameters.

1. Some applications of population algorithms

Today, many tasks in our life are somehow connected with the search for the optimal solution. Optimization problems are solved using various optimization algorithms. Traditional mathematical techniques for solving the optimization problems in real world problems may not find the optimum. In this regard heuristic optimization techniques (intelligent self-learning or population algorithms) have been represented. Since the 1960s, many heuristic algorithms have been devised that combine regulation and randomness [1]. Evolutionary algorithms based on a principle of survival of the fittest are genetic algorithms, evolution strategies, evolutionary programming and genetic programming. Simulation-based heuristic algorithms have great searching capacities and surmount some disadvantages of traditional mathematical methods. Some applications of the population algorithms:

- chemical-reaction optimization (a Pareto-based chemical-reaction optimization algorithm [2],
- the hybrid flow shop scheduling problem [3]),
- Bee algorithm (for prediction of heats of combustion of compounds [4]),
- problems for computing the probability of a given reaction sequence (algorithms for finding most-probable reaction sequences in stochastic chemical kinetic systems [5]),
- for efficient solution of population balance (optimization of batch crystallization processes [6]),
- for obtaining kinetic parameters in nonisothermal pyrolysis of biomass (evolutionary algorithms such as differential evolution [7]),
- optimization of industrial fluid catalytic cracking unit having five lump kinetic scheme, as well as development of a kinetic reaction model (genetic algorithm [8], [9], [10], [11]).

In this article we consider the phenomenon-mimicking metaheuristic Harmony Search algorithm (a relatively new population based meta-heuristic algorithm) is instigated by the improvisation process of jazz musicians and is presented by Zong Woo Geem, Joong Hoon Kim, and G. V. Loganathan in 2001 [12]. The Harmony search algorithm is an efficient evolutionary algorithm. In this analyzable algorithm a matrix of Harmony Memory is randomly generated. A new matrix of Harmony Memory is

generated by using all the solutions in the Harmony memory and if new solution is better than the previous solution in Harmony memory, the worst solution replaced by new solution. Harmony search algorithm creates a new vector after considering all existing vectors and Harmony search algorithm does not need the setting of initial values of variable. The Harmony search algorithm progressively enhances the fitness of the solution vector in an iterative fashion. These points help Harmony search algorithm in increasing flexibility and in searching better result. There four stages:

- initialization of the Harmony memory;
- improvisation of a new harmony;
- inclusion of the newly generated harmony in the Harmony memory (HM) provided that its fitness improves the worst fitness value in the previous Harmony memory;
- returning to step improvisation until a termination criteria (e.g. maximum number of iterations or fitness stall) is satisfied.

2. Harmony search method in the problem of chemical kinetics

The methods used to design the kinetic model are divided into methods for solving the direct and inverse problems of chemical kinetics. In most cases, chemical kinetics equations are sees of ordinary nonlinear differential equations (1) with initial conditions (2).

$$\frac{dx_i}{d\tau} = \frac{F_i - x_i F_N}{N}, i = 1,..., I,$$

$$F_i = \sum_{j=1}^{J} \nu_{ij} W_j, \frac{dN}{d\tau} = F_N = \sum_{j=1}^{J} \delta_j W_j, \delta_j = \sum_{i=1}^{I} \upsilon_{ij},$$

$$w_j = k_j^0 \cdot \exp\left(-\frac{E_j^-}{RT}\right) \cdot \prod_{i=1}^{M} x_i^{|\alpha_{ij}|} - k_{-j}^0 \cdot \exp\left(-\frac{E_j^+}{RT}\right) \cdot \prod_{i=1}^{M} x_i^{|\beta_{ij}|} \quad (1)$$

$$\tau = 0, x_i(0) = x_i^0, N = 1, \quad (2)$$

where I – the number of substances involved in the reaction; J – the number of stages; ν_{ij} – stoichiometric coefficients; E_j^-, E_j^+ – activation energy of direct and reverse reactions, *kal/mol*; R – gas constant, *kal/(mol·K)*; T – temperature, *K*; α_{ij} – negative elements of the matrix, β_{ij} – positive elements of the matrix; k_j^0, k_{-j}^0 – preexponential factors.

Differential equations in chemical kinetics are often stiff, and conventional methods (such as Runge-Kutta) are unacceptable. It was observed that it is better to solve them by implicit methods.

In this paper such methods of solving a direct kinetic problem as the Rosenbrock method, the Runge-Kutta method and the Geer method will be used. To determine the reaction rate constants and activation energies, the inverse problem of chemical kinetics will be solved, the solution of which is a multiple solution of the direct problem by iterating over the rate constants of the stages (or a set of preexponents and activation energies) by some algorithm. The problem of optimization, namely minimization of the functional (3) deviation of experimental data from the calculated ones, is posed:

$$F = \sum_{i=1}^{M} \sum_{j=1}^{N} \left| x_{ij}^{calc} - x_{ij}^{\exp} \right|, \quad (3)$$

where x_{ij}^{calc} – calculated values; x_{ij}^{exp} – experimental data; M – the number of experiment points; N – the number of substances involved in the reaction.

The inverse problem of chemical kinetics belongs to the problems of continuous global optimization. Features of such problems are often nonlinearity, undifferentiability, multiextremality (multimodality), lack of analytical expression and high computational complexity of optimized functions, as well as high dimensionality of the search space. These features of chemical kinetics problems explain the lack of a universal algorithm for their solution. In this paper, we consider a harmony search method, which is one of the population algorithms. All population algorithms belong to the class of heuristic algorithms, that is, algorithms for which convergence to a global solution is not proven, but it is experimentally established that in most cases they give a good enough solution.

Population algorithms of search optimization in comparison with classical algorithms have advantages, first of all, in solving problems of high dimension, multimodal and poorly formalized problems, which are inverse problems of chemical kinetics.

We are developing heuristic methods for solving inverse problems of chemical kinetics. Let's dwell on the method of harmonic search.

The improvisation procedure is mainly controlled by two different probabilistic operators, which are sequentially applied to each note so as to produce a new set of improvised harmonies or candidate solutions:

•The Harmony Memory set the probability that the new value for a certain element is drawn uniformly from the values of this same element in all the remaining vectors (random consideration).

•the new value x’ for a given element value x is obtained by adding a small random amount to the existing value x.x’=x+ωx·ε (ωx- the pitch bandwidth, and ε is a random number drawn from an uniform distribution with support [−1; 1].

The Harmony Search (HS) algorithm is able to solve a combinatorial or continuous problems [13]. Harmony Search algorithm can produce better solutions in less number of iterations [12]. The flowchart of the algorithm is shown in Fig. 1.

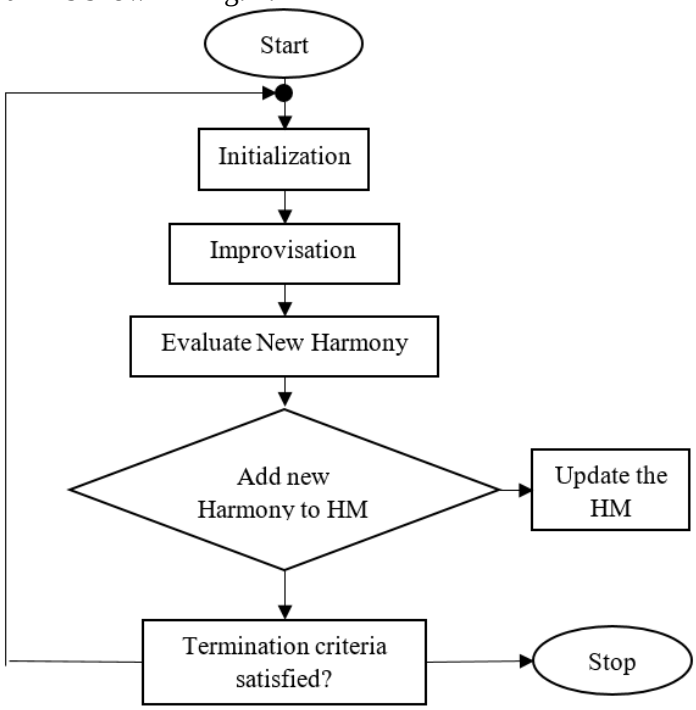

Figure 1. Flowchart of the HS algorithm [13].

The Harmony Search algorithm balances diversification and intensification. The Harmony Search algorithm is able to solve a combinatorial or continuous problems [13]. Harmony search algorithm have been revealed in varied applications: design of networks [14], load dispatch problem in electrical engineering [15], data mining [16].

The potential of the development of the Harmony search algorithm is huge. Optimization problems are often possible in chemical kinetics. A search for the application of the harmonic algorithm in chemical kinetics has shown that it is not widely used yet.

For instance, in work [17] the harmonic algorithm was used to improve the Alopex-based evolutionary algorithm for application in reaction kinetic parameter estimation. By compared with original Alopex-based evolutionary algorithm, the performance of the improved algorithm Harmony search Alopex-based evolutionary algorithm was tested on 22 unconstrained benchmark functions. The testing results show that Harmony search Alopex-based evolutionary algorithm clearly outperforms original Alopex-based evolutionary algorithm for almost all the benchmark functions.

Harmony search Alopex-based evolutionary algorithm is used to estimate reaction kinetic parameters for a heavy oil thermal cracking three lumps model and Homogeneous mercury (Hg) oxidation [17].

The results of testing some optimization algorithms showed that Harmony search algorithm in most cases were the cheapest (in terms of the number of iterations needed to achieve the desired level of suitability) [18].

The authors believe that work is needed for improving the simulation methodology (including new thermodynamic models, and the minimization of the Gibbs free energy), and on the development of approaches to enhance the reliability and reproducibility of this new variant of the Harmony Search algorithm [1].

3. Conclusion

Thus, the paper shows examples of the application of population algorithms in various studies. In particular, we focused on the study of the harmonic search algorithm. Population algorithms of search optimization in comparison with classical algorithms have advantages, first of all, in solving problems of high dimension, multimodal and poorly formalized problems, which are inverse problems of chemical kinetics. At the moment, we have presented the flowcharts of the harmonic search algorithm, and also formulated the problem of chemical kinetics. In the future, we plan to develop a program for the numerical simulation of a specific chemical process, based on the application of the described algorithm.

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5. References

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