OPTIMIZATION OF NON-LINEAR CHEMICAL PROCESSES USING EVOLUTIONARY ALGORITHM

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Abstract: This paper presents the application of Differential Evolution (DE), an Evolutionary Computation method, for the optimization of non-linear chemical processes. Two test problems (“Optimum fuel allocation in power plants” and “Optimization of drying process for a through-circulation dryer”), taken as case studies, are solved using DE. Comparison is made with traditional algorithm based on direct search and systematic search region reduction. It is found that DE, an exceptionally simple evolutionary algorithm, is significantly faster and yields the global optimum for a wide range of the key parameters.

Key Words: Optimization, Evolutionary Algorithm, Differential Evolution, Non-linear chemical processes, Direct search Method.

INTRODUCTION

The optimization of non-linear constrained problems is relevant to chemical engineering practice [Wong, (1990); Salcedo, (1992); Floudas, (1995)]. Non-linearities are introduced by process equipment design relations, by equilibrium relations and by combined heat and mass balances. The design variables may be floating points [non-linear programming (NLP) problems] or some of them may be integers [mixed integer non-linear programming (MINLP) problems].

In recent years, evolutionary algorithms (EAs) have been applied to the solution of NLP in many engineering applications. The best-known algorithms in this class include Genetic Algorithms (GA), Evolutionary Programming (EP), Evolution Strategies (ES) and Genetic Programming (GP). There are many hybrid systems, which incorporate various features of the above paradigms and consequently are hard to classify, which can be referred just as EC methods [Dasgupta and Michalewicz, (1997)]. They differ from the conventional algorithms since, in general, only the information regarding the objective function is required. In recent years, EC methods have been applied to a broad range of activities in process system engineering including modeling, optimization and control. Differential Evolution (DE), developed by Price & Storn [1997], is one of the best EC methods. This method provides one of the best genetic algorithms for solving the real-valued test function. The convergent speed of the DE is very high. In the present study, two test problems (“Optimum fuel allocation in power plants” and “Optimization of drying process for a through-circulation dryer”) are studied using DE, a hybrid evolutionary computation method. These problems arise from the area of chemical engineering, and represent difficult non-linear optimization problems, with equality & inequality constraints. Comparison is made with a direct search procedure (which utilizes pseudo random numbers over a region).

DIFFERENTIAL EVOLUTION (DE)

DE is an improved version of Genetic Algorithms (GA) [Deb, (1996)] for faster optimization. DE uses real coding of floating point numbers. Among the DE’s advantages are its simple structure, ease of use, speed and robustness. Price & Storn [1997] gave the working principle of DE with single strategy. Later on, they suggested ten different strategies of DE [Price and Storn, (2002)]. The strategy to be adopted for a problem is to be determined by trial & error. The key parameters of control are: NP - the population size, CR - the crossover constant, F - the weight applied to random differential (scaling factor).

The crucial idea behind DE is a scheme for generating trial parameter vectors. Basically, DE adds the weighted difference between two population vectors to a third vector. Price & Storn [2002] have given some simple rules for choosing key parameters of DE for any given application. DE has been successfully applied in various fields. The various applications of DE are: digital filter design [Storn, (1995)], fuzzy decision making problems of fuel ethanol production [Wang et al., (1998)], design

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of fuzzy logic controller [Sastry et al., (1998)], batch fermentation process [Chiou and Wang, (1999); Wang and Cheng, (1999)], multi sensor fusion [Joshi and Sanderson, (1999)], dynamic optimization of continuous polymer reactor [Lee et al., (1999)], estimation of heat transfer parameters in trickle bed reactor [Babu and Sastry, (1999)], optimal design of heat exchangers [Babu and Munawar, (2000); (2001)], synthesis & optimization of heat integrated distillation system [Babu and Singh, (2000)], optimization of non-linear functions [Babu and Angira, (2001a)], optimization of thermal cracker operation [Babu and Angira, (2001b)] etc. The DE algorithm used in the present study is reported elsewhere [Babu and Angira, 2002].

CASE STUDIES

Problem-1: Optimum Fuel Allocation in Power Plants.

The problem of minimizing the purchase of fuel oil (FO) is considered. In a power plant it is desired to produce an output of 50 MW from a two-boiler-turbine-generator combination (Fig. 1). It can use fuel oil or blast furnace gas (BFG) or any combination of these. The maximum BFG that is available is specified. By applying nonlinear curve-fitting Hovanessian & Stout [1963] obtained the fuel requirements for the two generators explicitly in terms of MW produced. For generator-1 the fuel requirements for fuel oil in tons per hour is given by the equation (1):

$$f_1 = 1.4609 + 0.15186x_1 + 0.00145x_1^2 \qquad (1)$$

and for BFG in fuel units per hour

$$f_2 = 1.5742 + 0.1631x_1 + 0.001358x_1^2 \qquad (2)$$

where x_1 is the output in MW of generator-1.

Similarly for generator-2 the fuel oil requirement is:

$$g_1 = 0.8008 + 0.2031x_2 + 0.000916x_2^2 \qquad (3)$$

and for BFG,

$$g_2 = 0.7266 + 0.2256x_2 + 0.000778x_2^2 \qquad (4)$$

where x_2 is the output in MW of generator-2.

Assumptions:

1. Only 10.0 units of BFG are available per hour.
2. Each generator may use any combination of fuel oil or BFG.
3. When a combination of fuel oil and BFG is used the effects are additive, i.e., if in generator-1 we use fuel oil and BFG in 1/3 ratio to produce x_1 MW, then the total fuel consumption consists of 0.25 f_1 tons of fuel oil per hour and 0.75 f_2 fuel units of BFG per hour.

The problem is to produce 50 MW from the two generators in such a way that the amount of fuel oil consumed is minimum. Mathematically, the problem can be formulated as follows:

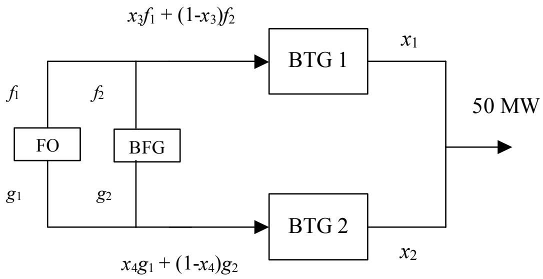

Fig. 1 Two-boiler-turbine-generator Power plant

Minimize $\qquad C = x_3 f_1 + x_4 g_1. \qquad (5)$

where f_1 and g_1 are given by equations (1) and (4) respectively.

Subject to

(a) Operating range for the generator-1:
$$18 \le x_1 \le 30 \qquad (6)$$
(b) Requirement of 50 MW of Power:
$$x_2 = 50 - x_1 \qquad (7)$$
(c) Operating range of generator-2
$$14 \le x_2 \le 25 \qquad (8)$$
(d) Fraction of fuel oil used in generator-1
$$0 \le x_3 \le 1 \qquad (9)$$
(e) Fraction of fuel oil used in generator-2
$$0 \le x_4 \le 1 \qquad (10)$$
(f) Availability of blast furnace gas (BFG)
$$\text{BFG} = (1 - x_3) f_2 + (1 - x_4)\, g_2 \le 10.0 \qquad (11)$$

where f_2 and g_2 are given by Equation (2) and (4) respectively.

Hence the problem is to choose the variables x_1, x_3, and x_4 so that C as given by equation (5) is minimized because the variable x_2 is eliminated by using equation (7). There are five inequality constraints embodied in equation (6) and equation (8) to (11). Also note that there is no lower limit restriction on equation (11) since computationally BFG cannot become negative.

Problem 2: Optimization of Drying Process for a Through-Circulation Dryer.

This problem deals with the maximization of the drying production rate in a through-circulation dryer [Chung, (1972)]. The drying production rate, in terms of the independent operating variables, is a non-linear objective function, and is optimized under the nonlinear inequality constraint function using DE. We use the data and corrected equations as in Chung [1972; 1973]. The problem is to find the mass flow rate x_1, and the bed thickness x_2 such that the drying production rate (P) is maximized. Mathematically, it can be expressed as follows:

Maximize P

$$P = 0.033x_1\left[\frac{0.036}{1-e^{107.9x_2/x_1^{0.41}}}+0.095-B\right]^{-1} \tag{12}$$

$$\text{where, } B = \frac{9.27\times10^{-4}x_1^{0.41}}{x_2}\ln\left(\frac{1-e^{-5.39x_2/x_1^{0.41}}}{1-e^{-107.9x_2/x_1^{0.41}}}\right)$$

Subject to the following constraints:

(1) Power constraint

$$0.2 - 4.62 \times 10^{-10}\, x_1^{2.85}\, x_2 - 1.055 \times 10^{-4}\, x_1 \geq 0 \tag{13}$$

(2) Pressure drop constraint

$$4/12 - 8.20 \times 10^{-7}\, x_1^{1.85}\, x_2 - 2.25/12 \geq 0. \tag{14}$$

(3) Drying time ratio constraint

$$0.64 - 109.6\frac{x_2}{x_1^{0.41}}\left[\frac{0.036}{1-e^{107.9x_2/x_1^{0.41}}}+0.095-B\right] \geq 0 \tag{15}$$

RESULTS AND DISCUSSION

For Problem-1, Hovanessian & Stout [1963] obtained the minimum fuel oil consumption of 3.17 tons/hour by using separable programming where the nonlinearities were approximated by linear sections and the problem was solved by the standard linear programming procedure. Luss and Jaakola [1973] obtained the minimum fuel consumption of 3.05 tons/hour by using the optimization procedure based on direct search and systematic search region reduction.

Chung [1973] solved the Problem-2 using differential algorithm and arrived at the maximum drying production rate (P) of 172.5 lb/ft^{2}hr, with x_1 = 975.6 lb/ft^{2}hr, and x_2 = 0.524 ft. Luss and Jaakola [1973] reported the maximum P of 172.49 lb/ft^{2}hr, with mass flow rate of 976.76 lb/ft^{2}hr & bed thickness of 0.5235 ft.

Table-1 shows the results obtained using DE with/without forcing the bound on variables, and Table-2 presents the comparison of DE with traditional method (Direct search method). The stopping criteria adopted for DE is to terminate the search process when one of the following conditions is satisfied: (1) the maximum number of generations is reached (assumed 1000 generations. (2) $| f^k_{\max} - f^k_{\min} | < 10^{-4}$ where f is the value of objective function for k-th generation. After the mutation & recombination, if the bound (i.e. lower & upper limit of a variable) is violated then it can be brought in the bound range (i.e. between lower & upper limit) either by forcing it to lower/upper limit (forced bound) or by randomly assigning a value in the bound range (without forcing). In Table-1 & Table-2, NFE & NRC represent respectively, the mean number of objective function evaluations and the percentage of runs converged to the global optimum in all the 10 executions (with different seed values). The key parameters used are F = 0.7; CR = 0.99.

It is interesting to note here that the value of F has a significant effect on convergence to optimal solution. It is found that DE did not converge to the same optimal solution using different seeds for F values less than 0.6. However, the CR (the crossover constant) has very little effect on optimal solution. In Problem-1 & Problem-2, NFE without forcing is slightly more than NFE with forced bound (Table-1). Also, the NRC with forced bound is not 100% in Problem-2 while NRC without forcing is 100% for both the problems.

Table 1. Results of DE (DE/rand/1/bin)

Prob -lem No.	PI with DE	DE (FB) (NRC/NFE/CPU-time$)	DE (Without forcing) (NRC/NFE/CPU-time$)
1	3.0522	100/3291/0.11 sec	100/3690/0.121 sec
2	172.487	80/1374/0.066 sec	100/1488/0.110 sec

$ Pentium III/500 MHz; PI=Performance Index; FB=Forced Bound.

Table-2 shows the comparison of DE (with forcing the bound) with traditional direct search method. They cannot be compared on the basis of CPU-time since the computer used is different in the each case. However the value of objective function i.e. the performance index is slightly better using DE as compared to direct search method. But the NFE are slightly less in case of direct search method (9.17 % & 3.7 % less than that of DE for problem-1 & 2 respectively).

Table 2. Results of DE & Direct search method (DSM).

Prob -lem No.	PI with DE	PI with DSM	DE (FB) (NFE/CPU-time$)	DSM (NFE/CPU -time*)
1	3.0522	3.0526	3291 / 0.11 sec	2989 /1 sec
2	172.487	172.47	1374 / 0.066 sec	1323 /5 sec

* IBM 370/165; PI=Performance Index
$ Pentium III/500 MHz

CONCLUSIONS

In the present study, two optimal design problems as case studies form chemical engineering area (“Optimum fuel allocation in power plants” and “Optimization of drying process for a through-circulation dryer”) have been solved using DE. Results indicate that the bound on variables, when violated, should not be forced to lower/upper limit. In such cases, assigning a random value between lower & upper limit found to give 100% convergence to global optimum. It is found that the performance of DE is better than that of traditional direct search method in finding the true global optima for nonconvex nonlinear problems.

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