A DIFFERENTIAL EVOLUTION APPROACH FOR GLOBAL OPTIMIZATION OF MINLP PROBLEMS

B.V. Babu and Rakesh Angira*

Department of Chemical Engineering
Birla Institute of Technology & Science
Pilani - 333 031 (Rajasthan) India

ABSTRACT

The global optimization of mixed integer non-linear programming (MINLP) problems is an active research area in many engineering fields. In this work, Differential Evolution (DE), a hybrid Evolutionary Computation method, is used for the optimization of nonconvex MINLP problems and a comparison is made among the algorithms based on hybrid of Simplex & Simulated Annealing (M-SIMPSA), Genetic Algorithms (GA), and DE. It is found that DE, an exceptionally simple evolutionary computation method, is significantly faster and yields the global optimum for a wide range of the key parameters. Results indicate that DE is more reliable, efficient and hence a better approach to the optimization of nonconvex non-linear problems. DE found to be the best evolutionary computation method in all the problems studied.

1. INTRODUCTION

A large number of process synthesis, design and control problems in Chemical Engineering can be modeled as mixed integer nonlinear programming (MINLP) problems [9, 10, 24]. They involve continuous variables and integers. Due to their combinatorial nature, these problems are considered to be difficult. Gradient optimization techniques have only been able to tackle special formulations, where continuity or convexity had to be imposed, or by exploiting special mathematical structures. Stochastic algorithms, also known as adaptive random search methods, have tackled MINLP problems, mostly in the area of Chemical Engineering [26]. There has been a growing interest in algorithms, which are based on the principle of evolution (survival of the fittest) since two decades. They are referred as Evolutionary Algorithms (EA) or Evolutionary Computation methods (EC methods). In recent years, EAs have been applied to the solution of MINLP problems 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). Also, 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 [11]. They differ from the conventional algorithms since, in general, only the information regarding the objective function is required.

Differential Evolution (DE) is one such technique that is exceptionally simple, fast and robust. It is basically a computerized search and optimization algorithm and is more likely to find a function's true global optimum.

So far various methods such as branch and bound technique [18], outer-approximation (OA)/equality-relaxation algorithm [14, 15, 16], variant of OA method [28], adaptive random-search method [26], branch-and-reduce algorithm [17], MINLP Simplex Simulated Annealing Algorithm (M-SIMPSA) [24], and genetic algorithm & evolution strategies [23] have been used for solving MINLP problems. In the present study, seven test problems are studied using DE. These are difficult non-convex optimization problems with continuous and discrete variables. Hence the optimization needs an efficient strategy in searching for the global optimum.

2. DIFFERENTIAL EVOLUTION (DE)

DE [21] is an improved version of GA [12] for faster optimization. Unlike simple GA that uses binary coding for representing problem parameters, 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 [21] gave the working principle of DE with single strategy. Later on, they suggested ten different strategies of DE [22]. A strategy that works out to be the best for a given problem may not work well when applied

*Corresponding Author: Professor of Chemical Engineering & Head of ET Department, ESD (Workshop), BITS, Pilani-333031. E-mail: bvbabu@bits-pilani.ac.in; Fax: +91-0159-7644183; Phone: +91-0159-7645073 Ext. 205

for a different problem. Also, the strategy and key parameters to be adopted for a problem are 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 detailed Differential Evolution algorithm used in the present study is given below:

- Choose a strategy
- Initialize the value of D (Number of independent parameters), NP, CR, F & gen_max.
- Initialize all the vector population randomly in the given upper & lower bound.
  For I=1 to NP
  {For j=1 to D
  x_{ij} = random Number}
- Evaluate the cost of each vector.
- Find out the vector with the lowest cost.
- Repeat
- Perform mutation & recombination.
  a) For each vector x_t (target vector), select three distinct vectors x_a, x_b & x_c (select five, if two vector differences are to be used) randomly from the current population (primary array) other than vector x_t.
  b) Perform crossover for each target vector with its noisy vector to create a trial vector.
- 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).
- Perform selection for each target vector, x_t by comparing its cost with that of the trial vector. Vector with lower cost is selected for next generation.
- Till termination criteria do not meet.
- Print results.

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 [22] 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 [27], batch fermentation process [13, 19], dynamic optimization of continuous polymer reactor [25], estimation of heat transfer parameters in trickle bed reactor [3], optimal design of heat exchangers [7, 8], synthesis & optimization of heat integrated distillation system [6], optimization of an alkylation reaction [1], scenario-integrated optimization of dynamic systems [2], optimization of non-linear functions [4], optimization of thermal cracker operation [5] etc.

3. CASE STUDIES

To illustrate the applicability of DE to the nonconvex MINLP problems, seven test problems proposed by different authors are solved. Problem-2 and Problem-4, with equality constraints were difficult to deal with. Hence, the problems are reformulated (as Problem-2* and Problem-4*) by eliminating the equality constraints and incorporating them in inequality constraints and/or in objective function thereby reducing the number of constraints and parameters.

Problem-1: This example has a non-linear constraint and has been proposed by Kocis & Grossmann [15]. It has also been solved by other authors [9, 17, 23, 24].

$$\text{Min } f(x, y) = 2x + y$$

Subject to

$$1.25 - x^2 - y \le 0$$
$$x + y \le 1.6$$
$$0 \le x \le 1.6$$
$$y \in \{0, 1\}$$

The global optimum is $(x, y; f) = (0.5, 1; 2)$.

Problem-2: This problem, with a non-linear constraint is proposed by Kocis & Grossmann [16] and also studied by few other authors [23, 24, 26].

$$\text{Min } f(x_1, x_2, y) = -y + 2x_1 + x_2$$

Subject to

$$x_1 - 2\exp(-x_2) = 0$$
$$-x_1 + x_2 + y \le 0$$
$$0.5 \le x_1 \le 1.4$$
$$y \in \{0, 1\}$$

The global optimum is $(x_1, x_2, y; f) = (1.375, 0.375, 1; 2.124)$.

Problem-2*: Problem-2 can be reformulated as follows:

$$\text{Min } f(x_1, y) = -y + 2x_1 - \ln(x_1/2)$$

Subject to

$$-x_1 - \ln(x_1/2) + y \le 0$$
$$0.5 \le x_1 \le 1.4$$
$$y \in \{0, 1\}$$

The global optimum is same as in Problem-2.

Problem-3: It presents a non-linear constraint. It was first studied by Floudas [10] and also solved by others [23, 24].

$$\text{Min } f(x_1, x_2, y) = -0.7y + 5(x_1 - 0.5)^2 + 0.8$$

Subject to

$$-\exp(x_1 - 0.2) - x_2 \le 0$$
$$x_2 + 1.1y \le -1.0$$

$x_1 - y \le 0.2$
$0.2 \le x_1 \le 1$
$-2.22554 \le x_2 \le -1$
$y \in \{0, 1\}$

The global optimum is $(x_1, x_2, y; f) = (0.94194, -2.1, 1; 1.07654)$.

Problem-4: It has been taken from Kocis & Grossmann [14]. The objective here is to select one between two candidate reactors in order to minimize the production cost. Also, it has been solved by others [23, 24, 28, 29].

$$\text{Min } f(x, y_1, y_2, v_1, v_2) = 7.5y_1 + 5.5y_2 + 7v_1 + 6v_2 + 5x$$

Subject to

$y_1 + y_2 = 1$
$z_1 = 0.9[1 - \exp(-0.5v_1)]\, x_1$
$z_2 = 0.8[1 - \exp(-0.4v_2)]\, x_2$
$z_1 + z_2 = 10$
$x_1 + x_2 = x$
$z_1y_1 + z_2y_2 = 10$
$v_1 \le 10y_1$
$v_2 \le 10y_2$
$x_1 \le 20y_1$
$x_2 \le 20y_2$
$x_1, x_2, z_1, z_2, v_1, v_2 \ge 0$
$y_1, y_2 \in \{0, 1\}$

The global optimum is: $(x, y_1, y_2, v_1, v_2; f) = (13.36227, 1, 0, 3.514237, 0; 99.245209)$.

Problem-4*: This can be reformulated without equality constraints as follows:

$$\text{Min } f(y_1, v_1, v_2) = 7.5y_1 + 5.5(1 - y_1) + 7v_1 + 6v_2 + 50\frac{1 - y_1}{0.8[1 - \exp(-0.4v_2)]} + 50\frac{y_1}{0.9[1 - \exp(-0.5v_1)]}$$

Subject to
$0.9[1 - \exp(-0.5v_1)] - 2y_1 \le 0$
$0.8[1 - \exp(-0.4v_2)] - 2(1 - y_1) \le 0$
$v_1 \le 10y_1$
$v_2 \le 10(1 - y_1)$
$v_1, v_2 \ge 0$
$y_1 \in \{0, 1\}$

The global optimum is same as in Problem-4.

Problem-5: This problem was studied by many authors [9, 17, 23, 24, 26]. It presents several nonlinear constraints.

$$\text{Min } f(x_1, x_2, x_3, y_1, y_2, y_3, y_4) = (y_1 - 1)^2 + (y_2 - 1)^2 + (y_3 - 1)^2 - \ln(y_4 + 1) + (x_1 - 1)^2 + (x_2 - 2)^2 + (x_3 - 3)^2.$$

Subject to

$y_1 + y_2 + y_3 + x_1 + x_2 + x_3 \le 5$
$y_3^2 + x_1^2 + x_2^2 + x_3^2 \le 5.5$
$y_1 + x_1 \le 1.2$
$y_2 + x_2 \le 1.8$
$y_3 + x_3 \le 2.5$
$y_4 + x_1 \le 1.2$
$y_2^2 + x_2^2 \le 1.64$
$y_3^2 + x_3^2 \le 4.25$
$y_2^2 + x_3^2 \le 4.64$
$x_1, x_2, x_3 \ge 0$
$y_1, y_2, y_3, y_4 \in \{0, 1\}$

The global optimum is $(x_1, x_2, x_3, y_1, y_2, y_3, y_4; f) = (0.2, 1.28062, 1.95448, 1, 0, 0, 1; 3.557473)$.

Problem-6: It is taken from Wong [20] and also studied by others [23, 24].

$$\text{Max } f(x_1, x_2, x_3, y_1, y_2) = -5.357854x_1^2 - 0.835689y_1x_3 - 37.29329y_1 + 40792.141.$$

Subject to
$a_1 + a_2y_2x_3 + a_3y_1x_2 - a_4x_1x_3 \le 92$
$a_5 + a_6y_2x_3 + a_7y_1y_2 + a_8x_1^2 - 90 \le 20$
$a_9 + a_{10}x_1x_3 + a_{11}y_1x_1 + a_{12}x_1x_2 - 20 \le 5$
$27 \le x_1, x_2, x_3 \le 45$
$y_1 \in \{78, \ldots, 102\}$, integer
$y_2 \in \{33, \ldots, 45\}$, integer

where a_1 to a_{12} are constants the values of which are given in [23].

The global optimum (for any combination of x_2, y_2) is: $(x_1, x_3, y_1; f) = (27, 27, 78; 32217.4)$.

Problem-7: This is a multi-product batch plant problem with M serial processing stages, where fixed amounts Q_i from N products must be produced. Many authors [15, 18, 23, 24, 26] studied this problem.

$$\text{Min } f = \sum_{j=1}^{M} \alpha N_j V_j^{\beta}$$

Subject to

$$\sum_{i=1}^{N} \frac{Q_i T_{Li}}{B_i} \le H$$
$V_j \ge S_{ij}B_i$
$N_j\, T_{Li} \ge t_{ij}$
$1 \le N_j \le N_j^u$
$V_j^l \le V_j \le V_j^u$
$T_{Li}^l \le T_{Li} \le T_{Li}^u$
$B_j^l \le B_j \le B_j^u$

where, for the specific problem considered, $M = 3$, $N = 2$, $H = 6000$, $\alpha_j = 250$, $\beta_j = 0.6$, $N_j^u = 3$, $V_j^l = 250$ and $V_j^u = 2500$. The values of T_{Li}^l, T_{Li}^u, B_j^l and B_j^u are given by:

$T_{Li}^l = \max t_{ij}/N_j^u$
$T_{Li}^u = \max t_{ij}$
$B_j^l = Q_i * T_{Li}/H$

$B_j^u = \min(Q_i, \min_j V_j^u/S_{ij})$

The values of S_{ij} and t_{ij} [i = 1 to 2 (rows); and j = 1 to 3 (columns)] are reported in [23].

The global optimum is: (N_1, N_2, N_3, V_1, V_2, V_3, B_1, B_2, T_1, T_2; f) = (1, 1, 1, 480, 720, 960, 240, 120, 20, 16; 38499.8).

4. RESULTS AND DISCUSSION

Table-1 shows the results obtained using DE with/without forcing the bound on variables, and Table-2 presents the comparison of DE with GA & M-SIMPSA. 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 5000 generations for Problem-7 & 1000 generations for other problems). (2) $| f_{\max}^{k} - f_{\min}^{k} | < 10^{-5}$ 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).

In Problem-1 & Problem-2, NFE without forcing is slightly less than NFE with forced bound (Table-1). However, for other problems NFE with forced bound is significantly less than NFE without forcing. Also, the NRC with forced bound is not 100% in problems 2*, 3, 5 & 7 while NRC without forcing is 100% for all the problems. It is important to note that in Problem-3, NRC with forced bound is zero. It is because when upper limit of bound is violated, the value of variable is forced to the upper limit that resulted in convergence to non-optimal solution. However, for Problem-7, the NRC is 70% for forced bound and 10% without forcing the bound.

Table-2 shows the comparison of DE (without forcing the bound) with GA & M-SIMPSA. The NFE in DE is less than 11% of that in GA for all the problems (The range is 3% to 10.15% to be precise). However, for Problem-7, only DE is converging, while GA and M-SIMPSA are not converging to global optimum. Similarly, the NFE in DE ranges from 3.88% to 66.33 % of that in M-SIMPSA. Therefore, it is evident that DE took least NFE and maximum NRC to achieve global optima in each of the above test problems. It may be noted that GA could not converge to global optimum, while execution was reported to be halted in M-SIMPSA for Problem-7. Hence the performance of DE proved to be better than that of GA & M-SIMPSA in optimizing the mixed integer nonlinear programming problems considered in the present study.

Table-1. Results of DE[1]

Problem No.	DE[1] NFE/NRC (Forced bound)	DE[1] NFE/NRC (Without forcing)	Key parameters of DE[1] (NP/CR/F)
1	424/100	402/100	10/0.7/0.5
2*	442/80	410/100	10/0.9/0.7
3	352**/0	4346/100	20/0.8/0.7
4*	580/100	1416/100	20/0.8/0.5
5	9348/80	10425/100	30/0.6/0.9
6	414/100	3542/100	20/0.8/0.5
7	196786/70	222400/10	100/0.8/0.3

DE[1] Strategy used is DE/rand/1/bin (Price and Storn, 2002)
** Converged to a non-optimal solution
NFE = NP (1 + Number of generations)

Table-2. Comparison of DE[1], GA & M-SIMPSA

Problem No.	NFE/NRC (GA)	NFE/NRC (M-SIMPSA)	NFE/NRC (DE[1])
1	6787/100	607/99	402/100
2*	13939/100	10582/83	410/100
3	107046/90	#/0	4346/100
4*	22489/100	14738/100	1416/100
5	102778/60	22309/60**	10425/100
6	37167/100	27410/87	3542/100
7	225176/0	#/0	222400/10

Execution halted

5. CONCLUSIONS

Seven chemical engineering case study problems have been solved using DE in the present work. 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. Also there was difficulty in dealing with equality constraints (Problem-2 and Problem-4). However, when reformulated by eliminating these equality constraints, the algorithm exhibited 100% convergence. It is found that NFE is the least and NRC is highest in DE as compared to GA & M-SIMPSA. The performance of DE proved to be the best among the three population based methods for all the problems studied.

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