Box-Complex Assisted Genetic Algorithm for Optimal Control of Batch Reactor ⋆

Narendra Patel * **Nitin Padhiyar** **

* *Chemical Engineering Department, Vishwakarma Government Engineering College, Chandkheda, Ahmedabad-382424, Gujarat, India. (e-mail: narendra@iitgn.ac.in)*
** *Department of Chemical Engineering, Indian Institute of Technology Gandhinagar, Ahmedabad-382424, Gujarat, India. (e-mail: nitin@iitgn.ac.in)*

Abstract: To enhance convergence property of Genetic Algorithm (GA), we in this work propose modification in GA by combining the global search property of GA with a convergence property of Box-Complex method. Using the current population of GA, new members are created using Box-Complex concept, which replaces equal number of worst population members. A comparative study of the proposed GA with the conventional GA and widely accepted Jumping Gene GA (JG GA) is presented in this work. We have considered two mathematical and a batch reactor optimal control applications for evaluating the efficacy of the proposed GA. There are two user defined parameters in the proposed algorithm, namely extent of Box-Complex Assistance(BCA), and expansion/contraction factor α. Effect of both these parameters on convergence is presented in this work for the proposed GA.

Keywords: optimal control, Genetic Algorithm, Box-Complex method, batch reactor, off-line optimization

1. INTRODUCTION

Genetic Algorithm (Goldberg, 1989; Holland, 1975) is a popular stochastic optimization technique for past couple of decades and has been successfully applied to numerous applications of single and multi-objective optimization problems . Genetic Algorithm (GA) is more computationally expensive algorithm compare to the gradient based algorithms, but it is suitable for complex functions and more flexible.

There has been a significant contribution in GAs for past two decades mainly addressing the two aspects of a GA, namely 1) increasing convergence rate or reducing computational efforts and 2) maintaining or increasing the diversity among population members for enhancing the probability of obtaining global optimum solution. The conventional GA includes initialization, fitness assignment, fitness selection, crossover, mutation and survival selection as common steps. Crossover and mutation operators add diversity in the population leading to high probability of convergence to global optimum solution, selection method guides the GA to achieve appropriate convergence.

Usually hybridization of GA is done to combine the global search capacity of GA with efficient local search method to improve convergence rate without deteriorating the global search capacity. Pandey et al. (2014) presents an exhaustive review of different approaches implemented to prevent premature convergence with their strengths and weaknesses. El-mihoub et al. (2006) has reviewed different forms of integration between GAs and other search and optimization techniques. It was observed in hybridization of GAs that combination of a GA and a local search method can speed up the search to locate the exact global optimum. GA and Box-Complex method both being population based techniques, mixing their capabilities to develop more powerful hybrid technique is easy to implement. Applying a local search to the solutions that are guided by a GA to the most promising region can accelerate convergence to the global optimum. Hybridisation of gradient based technique with GA can potentially provide faster convergence. Usually these gradients are computed numerically when the analytical gradients are not available, which adds computational cost and numerical error as well. On the other hand Box Complex technique is a population based technique like GA. Hence, the hybridization is quite straightforward without significant additional computational efforts. To implement this concept, we propose a modification in GA by incorporating convergence property of Box-Complex method in GA. A related work on hybrid GA using Box Complex method by the authors can be found elsewhere (Patel and Padhiyar, 2015). Though, the choice of Complex, the results, and two test applications in this work are entirely different from the previous work.

The proposed modification for Box-Complex Assisted GA is discussed in next section. The two mathematical applications followed by the results and discussion are presented in Section 3. The proposed GA is then applied to an optimal control problem in a batch reactor in Section 4. The reported values in the open literature using other optimization algorithms for this application have also been

⋆ IIT Gandhinagar, Ahmedabad, Gujarat, India presented in this section. Finally the concluding remarks are presented in Section 5.

2. BOX-COMPLEX ASSISTED GENETIC ALGORITHM (BCA GA)

Box (1965) proposed a multi-start optimization method, which gives progressive convergence with significantly small population size compared to other population based evolutionary techniques such as GA. But this method has a limitation of getting trapped in local minima. To overcome the large computational effort with larger population for obtaining global minimum, we propose to combine global search property of GA; assisted by convergence property of Box-Complex method. One or more new members are created using the current population by Box-Complex concept at every generation. We add the new member(s) at every generation by replacing equal number of the inferior member(s) of the population, thereby maintaining the constant population size. Since the GA is a very popular optimization technique, we skip the detailed description of the conventional GA. The proposed modified GA with Box Complex Assistance is presented in next subsection.

2.1 Proposed Algorithm of BCA GA

We propose to modify the GA to incorporate the convergence capability of the Box-Complex method. Please note that eliminating step 6 from the proposed algorithm leads to the conventional GA. A stepwise implementation of the proposed GA modified for Box-Complex Assistance is as follows:

(1) Initialization:
- *Define system parameters such as number of variables, lower and upper bounds on decision variables.*
- *Specify GA parameters such as population size (Np), number of generations, parameters for GA operators and choice for BCA assistance.*

(2) Generation of Initial Population
- *Generate initial population of size Np, satisfying the bound constraints.*
- *Compute the fitness values of the all initial population members.*

(3) Crossover and Mutation
- *Carry out the crossover operation with user defined crossover probability.*
- *Carry out the mutation operation for the population generated after crossover.*

(4) Fitness calculation
- *Calculate fitness values of the child population generated after crossover and mutation.*

(5) Elitism selection
- *Select the Np best individuals from the pool of parent and child population(s) for the next generation.*

(6) Box-Complex Assistance
- *Select complex members as the best $n+1$ members from newly created population, where $n+1$ is the number of variables.*
- *Generate a new member by Box-Complex assistance, taking the projection of the worst member of complex through centroid of the remaining members of complex. The explanation on how to generate a new complex member using Box-Complex method from a given population is illustrated in next subsection.*
- *Calculate fitness value of the newly created BCA member and replace the worst member in the population if it is inferior to the BCA member.*
- *If the new member is inferior to the worst member in the population, move half way towards the centroid of remaining complex members.*
- *Calculate fitness value of the shifted member and replace the worst member in the population if it is inferior to the new member, else ignore the BCA member.*
- *In case of more than one BCA members ($BN > 1$), select best first n members and one $(n + BN)th$ member. This selection will skip previously used $(n+1)th$ members from the population. Follow the procedure adapted in previous steps until the total BN members are created.*

(7) Continuation of loop
- *This completes one loop. Stop if the convergence criteria is satisfied else go to step 3. Convergence criteria can be the maximum number of generations or tolerance in fitness value of the best member of the population.*

As can be noticed in the above BCA GA, there are two user defined parameters, namely number of BCA members, BN and the expansion/contraction factor, α. Small values of BN may contribute little to the convergence rate, maintaining high diversity created by crossover and mutation operators. On the other hand large BN values may increase the convergence rate at a cost of the population diversity. This may result in convergence to the local minima. For smaller values of the second tuning parameter, expansion/contraction factor (α) may not provide sufficient projection of the worst complex member in the direction of improvement. On the other hand very large value of α may lead to excessive projection of the worst complex member and consequently rejection of the new point. The process of generation of BCA member is illustrated in next subsection.

2.2 Illustration of Box-Complex Assistance

A Complex is created by selecting k members from population, where $k = n + 1$. The complex comprising of three points, A,B and R is shown in Fig. (1). The objective function values (Rosenbrock's function, 1) are evaluated for each vertex of the complex and are shown in table (1). The vertex (R) having the most inferior value of objective function is projected through the centroid of the remaining points(A and B) of complex. Centroid is calculated using the formula given at (2). The new point is obtained by projecting the worst vertex(R) through centroid at a distance α times the distance of the centroid from the rejected vertex. The new BCA member is calculated using (3). The process of generating a new vertex point in two dimensional space is graphically illustrated in Fig. (1) and values are presented in table 1 for α=0.8.

$$f = 100(x_2 - {x_1}^2)^2 + (1 - {x_1}^2)^2 \tag{1}$$

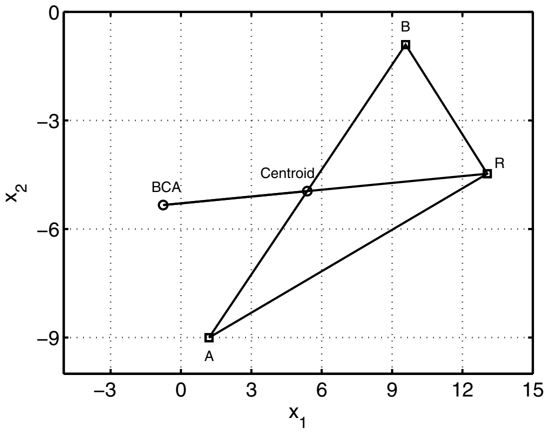

Fig. 1. Box-Complex method: Illustration of projection of worst vertex through centroid

$$x_{i,M} = \frac{1}{k-1}\left(\sum_{j=1}^{k} x_{i,j} - x_{i,R}\right) \quad (2)$$

$$x_{i,N} = \alpha(x_{i,M} - x_{i,R}) + x_{i,M} = (1+\alpha)x_{i,M} - \alpha x_{i,R} \quad (3)$$

3. NUMERICAL APPLICATIONS

For testing the efficiency and effectiveness of the proposed modified GA, we are using two mathematical test applications with known optimal solution.

3.1 Application 1

This unconstrained mathematical system (SUN et al. (2013), Rajesh et al. (2001) and Luus and Okongwu (1999)) has been used as a dynamic optimization problem for assessing the algorithm performance. The detailed mathematical model is formulated as,

$$min\, J(u) = x_2(t_f) \quad (4)$$

$$s.t.\ \frac{dx_1}{dt} = u,\ \frac{dx_2}{dt} = x_1^2 + u^2, \quad (5)$$

$$x(0) = [1, 0]^T,\ \ t_f = 1 \quad (6)$$

The application has a known global minimum analytical solution (LIU et al., 2013) as follows,

$$u^* = -2\frac{2e}{1+e^2}\sinh(1-t) \quad (7)$$

$$J^*_{min} = \frac{e^2-1}{1+e^2} \quad (8)$$

Note that for $t_f = 1$ h, the global minimum is found to be 0.761594.

Table 1. Illustration of BCA member calcaulation using Rosenbrocks function

Point	x_1	x_2	f
A	1.1970	-9.0043	15.2420
B	9.5731	-0.9029	16.6219
R	13.0600	-4.4721	18.9063
Centroid	5.3851	-4.9536	14.5029
BCA	-0.7549	-5.3387	12.6089

3.2 Application 2

The second test application along with the known optimum solution (SUN et al., 2013) is described as follows,

$$min\, J(u) = \frac{1}{2}\int_0^1 (x^2 + u^2)\, dt \quad (9)$$

$$s.t.\ \frac{dx}{dt} = -x + u,\ x(0) = 10,\ t_f = 1 \quad (10)$$

$$u^*(t) = 0.10(\sqrt{2}+1)\exp(\sqrt{2}t) - 9.9(\sqrt{2}-1)\exp(-\sqrt{2}t) \quad (11)$$

Note that at $t_f = 1$ h, the J^* is 19.2910.

3.3 Result Discussion

Real coded GA program developed in MATLAB 2011 is used in this work. The conventional GA code developed uses stochastic remainder roulette wheel selection, Simulated Binary Crossover (SBX) and Non-uniform mutation with elitism survival selection. The BCA GA code uses the same operators along with BC member addition as per the proposed algorithm. The Real coded JG GA is implemented using the same GA operators and JG operator as recommended by Nawaz Ripon et al. (2007). The GA parameters used for all the applications are summarized in table (2)

Table 2. GA parameters for Application 1(A1), Application 2(A2) and Batch Reactor(BR)

Parameter	A1	A2	BR
Number of decision variables	10	10	40
Lower limit(for all variables)	-15	-15	298
Upper limit(for all variables)	15	15	398
Population size	50	50	200
Number of generations	150	150	400
Crossover probability	0.9	0.9	0.9
Mutation probability	0.2	0.2	0.2
SBX crossover parameter, c	2	2	2
Non-uniform mutation parameter, b	4	4	4
JG probability	0.4	0.4	0.4
Box-Complex projection factor, α	0.9	0.9	0.9

For the previously discussed two test applications effect of Box-Complex Assistance (BCA) is tested for real coded GA and compared with conventional GA and Real coded Jumping Gene (JG) GA. We study sensitivity of both the tuning parameters for proposed GA, namely 1)extent of Box-Complex Assistance (BCA) and 2) expansion-contraction parameter α using these test applications. The extent of BCA represents the number of BCA members,BN used in evolution. We use BN value of 1 to 5 naming it as 1BCA to 5BCA. As GA is a stochastic optimization technique, it does not converge to the same solution every time even with the same initial population. Hence, we carry out ten simulation runs for every combination of the test application with different initial population. Please note that in BCA GA, extra function evaluations are carried out that of the BCA. Hence, we have shown convergence plot as a function of Number of Function Evaluations (NFEs) instead of generation number for computational efforts by various GAs.

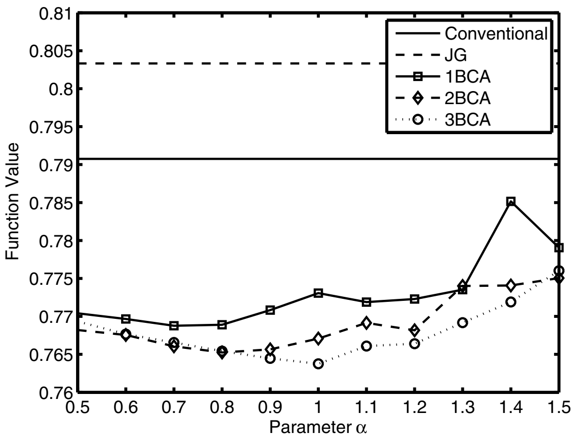

Fig. 2. Effect of expansion/contraction factor α on convergence at the end of 5000 NFEs for application 1 (average of ten runs)

The effect of tuning parameter α for application 1 is shown in Fig.(2). It is observed that BCA GA with α in the range of 0.5 to 1.5 always convergences to a better objective value. The best value of α for 1BCA and 2BCA cases is 0.8 and for 3BCA case it is 1.0. The statistical analysis of ten simulation runs at the end of 5000 NFEs are summarised in table(3). The best vale of 0.7621 close to the analytical solution of 0.7615 is achieved by 3BCA and 5BCA GAs. Standard deviation values clearly reflect that all BCA GA converges consistently better than conventional and JG GAs.

Table 3. Statistical analysis of ten simulation runs for application 1 at the end of 5000 NFEs

GA Type	Worst	Best	Average	Std. dev
Conventional	0.8106	0.7666	0.7908	0.0149
1BCA	0.7795	0.7657	0.7708	0.0052
2BCA	0.7680	0.7637	0.7657	0.0015
3BCA	0.7667	0.7621	0.7645	0.0015
4BCA	0.7667	0.7622	0.7640	0.0015
5BCA	0.7642	0.7621	0.7631	0.0008
JG	0.8223	0.7794	0.8033	0.0140

The Convergence profile for application 1 as the average of ten simulation runs has been shown in Fig.(3). The convergence rate of both the BCA GAs has been found to be significantly better than the other two GAs. At the end of 2000 NFEs objective function value obtained by 1BCA GA is obtained by conventional and JG GA after 3000 NFEs. Similarly, the function value of 1 obtained at 2000 NFEs by 2BCA GA, is obtained nearly after 4000 NFEs by conventional and JG GAs.

The effect of the other tuning parameter, namely expansion/contraction factor, α for application 1 is shown in Fig. (4). Note that too small value of α may not provide sufficient improvement in the newly created member, too large value may lead to infeasible member. Following this trend, the best value of α for 1BCA case is 0.8, for 2BCA case is 0.8 and 1.1, and for 3BCA case it is 1.1. The statistical analysis of ten simulation runs at the end of 5000 NFEs are summarized in table (4). The best objective function vale of 19.2907 is found to be marginally better than the reported value of 19.2910 by 4BCA GA. Standard

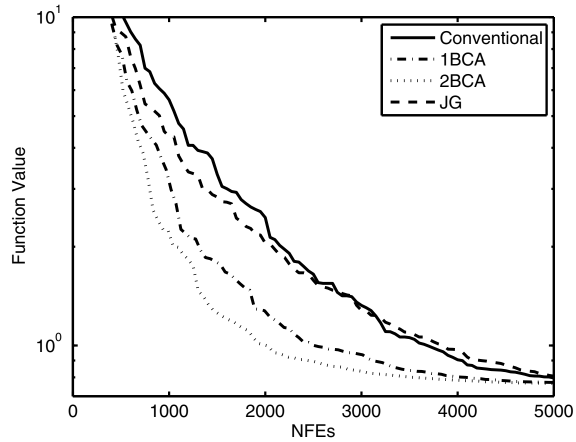

Fig. 3. Convergence profile for application 1 (average of the ten runs)

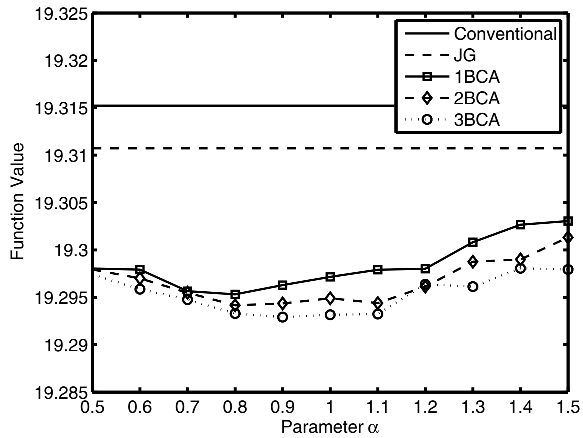

Fig. 4. Effect of expansion/contraction factor α on convergence at the end of 5000 NFEs for application 2 (average of ten runs)

deviation values clearly reflect that all BCA GA converges consistently better than conventional and JG GAs.

Table 4. Statastical analysis of ten simulation runs for application 2 at the end of 5000 NFEs

GA Type	Worst	Best	Average	Std. dev
Conventional	19.3251	19.3081	19.3152	0.0057
1BCA	19.2989	19.2928	19.2963	0.0019
2BCA	19.2975	19.2921	19.2944	0.0019
3BCA	19.2969	19.2913	19.2929	0.0017
4BCA	19.2989	19.2907	19.2940	0.0032
5BCA	19.2942	19.2912	19.2925	0.0010
JG	19.3229	19.3022	19.3107	0.0067

Convergence profiles as average of ten simulation runs has been shown in Fig.(5) for application 2. The convergence rate is significantly better for both the BCA GAs compared to the conventional and JG GAs. The objective function value obtained by both the BCA GAs at about 1500 NFEs is obtained after 2500 NFEs using conventional and JG GA. Though, after 5000 NFEs, all the GAs converge to the objective function values very close to each other.

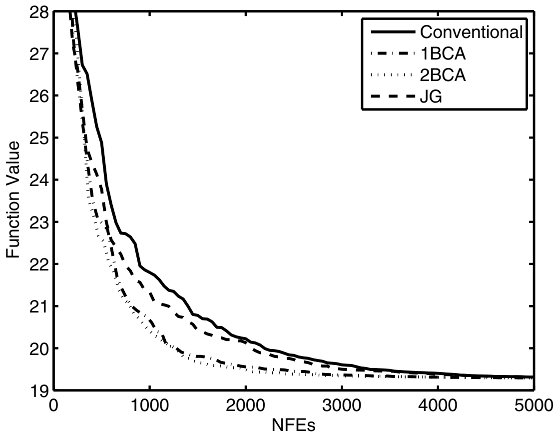

Fig. 5. Convergence profile for application 2 (average of the ten runs)

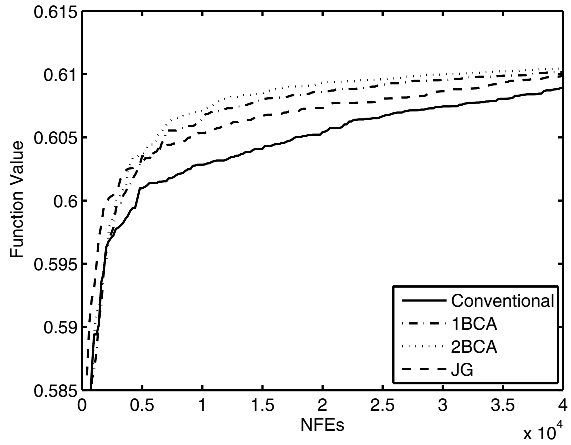

Fig. 6. Convergence profile for batch reactor application (average of the ten runs)

4. OPTIMAL CONTROL OF BATCH REACTOR

While the earlier two studies were the mathematical applications of dynamic optimization, we now present an off-line optimal control application of a batch reactor with reaction scheme, $A \rightarrow B \rightarrow C$ to optimize temporal temperature recipe for maximizing the yield of product B at the end of the batch time of 1 hour.

The optimal control problem for batch reactor is,

$$max\, J(T) = C_B(t_f) \tag{12}$$

$$s.t.\ \frac{dC_A}{dt} = -4000 \exp\left(\frac{-2500}{T}\right) C_A^2 \tag{13}$$

$$\begin{aligned}\frac{dC_B}{dt} = &\ 4000 \exp\left(\frac{-2500}{T}\right) C_A^2 \\ &-6.2X10^5 \exp\left(\frac{-5000}{T}\right) C_B\end{aligned} \tag{14}$$

$$[C_A^{(0)} C_B^{(0)}] = [10];\ 298 \leq T \leq 398 \tag{15}$$

4.1 Optimal Control Results for Batch Reactor

Generation wise convergence for batch reactor application are shown in Fig.(6). Unlike previous two applications, initial convergence rate of JG GA is higher than that of the conventional both the BCA GAs. Note that while the cost of extra function evaluation for BCA GA paid off for improved convergence, a shift of the convergence profile to the right has been observed. Though, after about 500 NFEs, the convergence rate is observed to be hindered by enhanced diversity provided by the JG GA on the convergence rate. On the other hand both the BCA Gas provide more convergence because of the Box-Complex Assistance. Further, at the end of 2000 NFEs, a tendency of further convergence is observed in case of the BC GAs, which is not found in the conventional and JG GAs. This can be attributed to the progressive convergence obtained by the Box Complex concept. The function value obtained at 40,000 NFEs by conventional GA is obtained by JG GA in about 30,000 NFEs. On the other hand 1BCA GA takes about 20,000 NFEs and 2BCA GA needs only 15,000 NFEs for the same convergence.

A comparative average convergence at the end of 40,000 NFEs for all GAs are shown in Fig.(7). The comparative graphs show that all BCA GAs converged to optimal solutions better than conventional and JG GAs. Also, it can be noted that all BCA GAs converged to very close optimal solutions, hence the plot is almost horizontal line connecting 1BCA to 5BCA points. The statistical analysis of ten simulation runs at 40,000 NFEs for all types of GAs are presented in table (6).

Table 5. Best objective function values for batch reactor application obtained by different contributors

Sr. No.	Algorithm/Method	Value	Reported by
1	Piecewise constant controls	0.610	Renfro et al. (1987)
2	Iterative Dynamic Programming (IDP)	0.61079	Luus (1994)
3	Two-point collocation	0.610767	Logsdon and Biegler (1989)
4	Relaxed reduced space SQP strategy	0.610775	Logsdon and Biegler (1993)
5	IDP with absolute error penalty functions	0.610775 (n=80)	Dadebo and Mcauley (1995)
6	Iterative Ant-Colony Algorithm (IACA)	0.6104 (n=20)	Zhang et al. (2005)
7	Complex Ant Colony Algorithm (CACA)	0.61045	Rajesh et al. (2001)
8	Hybrid Improved Genetic Algorithm (HIGA) with local search after 28000 NFEs.	0.61046 (n=20)	SUN et al. (2013)
9	Box-Complex Assisted GA (4BCA GA) after 40,000 NFEs	0.61092	this work

Table 6. Statastical analysis of ten simulation runs for batch reactor application at the end of 40,000 NFEs

GA Type	Best	Worst	Average	Std. dev
Conventional	0.60936	0.60859	0.60894	0.00027
1BCA	0.61045	0.61004	0.61022	0.00012
2BCA	0.61086	0.61016	0.61049	0.00021
3BCA	0.61075	0.61026	0.61046	0.00015
4BCA	0.61092	0.61020	0.61050	0.00018
5BCA	0.61078	0.61040	0.61051	0.00011
JG	0.61034	0.60958	0.60989	0.00023

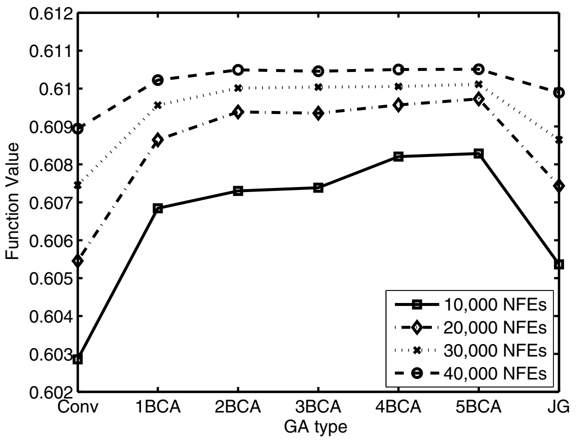

Fig. 7. Comparison of progressive convergence of conventional, 1BCA to 5BCA and JG GAs for batch reactor application (average of the ten runs)

Many researchers have worked on this application as a test bed for optimal control problem. The outcome of their work has been summarized in table (5). The best objective function value of 0.61079 has been obtained among these studies by Luus (1994) using iterative dynamic programming. Please note that the maximum concentration of B obtained in this study is 0.61092 for 4BCA GA after 40,000 NFEs, which is marginally better than the value reported by Luus (1994).

5. CONCLUSION

A Box-Complex method assisted GA is proposed in this work for enhancing the convergence rate for dynamic optimization problems. The member generated using Box-Complex method replaces the worst members of population. There are two user defined parameters, namely number of BC members, and expansion/contraction factor, α. This concept was extended for one to five members (1BCA to 5BCA) in GA and the GA results are compared with conventional GA and one of the widely accepted GA, namely JG GA. Also the sensitivity study of the other parameter, α has been presented. Two mathematical applications with known optimal profile are considered for the performance study and analysis of proposed GA. Optimal control of a batch reactor is a test application considered in the study, where the objective is to find optimal temperature profile to maximise the endpoint product concentration in a batch reactor at the end of one hour.

In all the three applications, convergence rate and the objective function values are compared for all GAs considered. Please note that extra function evaluation is carried out for every BCA member. Therefore, convergence profiles for various GAs are compared in terms of NFEs instead of generation. We notice that BCA GAs minimize computational effort significantly for all the three applications of optimal control problems. The authors recommend 2-3 number of BCA members and an α value of 0.8-1.3 for any application, which has consistently provided better results than the conventional and JG GAs in this work.

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