STUDY OF EFFECT OF CRO (CHEMICAL REACTION OPTIMIZATION) PARAMETERS ON OPTIMAL SOLUTIONS USING NUMERICAL EXPERIMENTATION

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ABSTRACT
Optimization of engineering operations is still a challenging task due to the non-linear and discontinuous target functions. The conventional methods lack in generic approach and hence methods based on nature-inspired evolutionary algorithms have been viewed as an alternative. Chemical Reaction Optimization is one of them. In a chemical reaction, the reactants are formed into products i.e. the unstable substances into optimally stable ones by undergoing four types of transformations. These steps became the source of inspiration in development of CRO algorithm. The optimal solution obtained using CRO is dependent upon its parameters. Present work aims at improving its performance by optimizing them. CRO program is developed in C++ & numerical experimentations have been conducted for two nonlinear functions involving two and three variables respectively. Combinations of the various CRO parameters such as population size, molecoll, KE loss rate, β and α have been chosen and the optimal values obtained are compared to decide the optimal structure of 'CRO'. The optimal structure of CRO parameters decided is applied in obtaining optimal solutions of these objective functions and the obtained values are compared with the optimal values reported in literature using conventional methods. It can be concluded that CRO has potential of providing optimal solution with matching or improved performance when compared to conventional methods similarly the present work has provided optimal combination of governing parameters of CRO with improved performance and short machine time.

KEYWORDS: *Optimization, CRO, Chemical reactions, optimal parameters, nonlinear functions*

I. INTRODUCTION

Nature being supreme has always been a source of inspiration to mankind. Researchers have constantly been trying to study and imitate some of the features of several natural processes. Evolutionary algorithms are a typical example of the same having applications in modelling, simulation and optimization of processes.[1]
Optimization is a phenomenon employed in the selection of the right combination of parameters from amongst a set of available alternatives. Engineering optimization problems are complex involving either maximization or minimization of a function value by choosing appropriate values of the input parameters from within an allowed set, range or constraints.[2] Whenever a large number of parameters decide the function value the optimal solution search becomes more and more complex and many conventional methods fail to address them.
Natural computing is a terminology introduced to encompass three classes of methods: 1) those that take inspiration from nature for the development of novel problem-solving techniques; 2) those that are based on the use of computers to synthesize natural phenomena; and 3) those that employ natural materials (e.g., molecules) to compute. [3]

Chemical Reaction Optimization is a nature inspired algorithm that is useful in operating solutions to various optimization problems. [4]

The paper is presented in sections starting with introduction to natural computing and optimization followed by introduction to Chemical Reaction Optimization and inspiration behind developing the CRO algorithm. In the next section the development procedure of program is discussed along with various components and features of the program. Details of the numerical experiments, its observations and the comparison of various parameters of CRO in obtaining optimal solutions is discussed at length. The paper concludes with highlighting the findings of present work & indicating the possible areas that need to be explored further.

II. INSPIRATION

A chemical reaction takes place when molecules of two species having different energy levels are contacted in a reactor. The basic principle of conversion of units of these species into another species is based on the principle of minimum total potential energy which asserts that a structure or body shall deform, displace or acquire a position that minimizes the total potential energy. The tendency to attain minimum total potential energy is due to second law of thermodynamics which states that the entropy of a system will maximize at equilibrium. Several possibilities emerge during this phenomenon that include on wall ineffective collision, decomposition of a molecule, inter-molecular ineffective collision and synthesis. These features have been imbibed in development of CRO algorithm. [5]

III. DEVELOPING CRO

Figure 1 shows the algorithm used to develop CRO. The details of various functions and parameters are as given below.

2.1 Basic components, elementary reactions, and concepts

In CRO the manipulated agents are molecules. Each molecule has several attributes, which are essential to the basic operations of CRO. The essential attributes are defined as follows:

1. **Molecular structure (ω)**: It captures a possible solution of the problem.
2. **Potential energy (PE)**: It represents the objective function value of the corresponding solution represented by ω. If 'f' denotes the objective function, then $PE\omega = f(\omega)$.
3. **Kinetic energy (KE):** It is a non-negative number and is specified initially and it is the tolerance of the system accepting the worst solution.
4. **Number of hits**: When a molecule undergoes a collision, one of the elementary reactions will be triggered and may experience a change in its molecular structure. Num-Hit is a record of the total number of hits (i.e. collisions) a molecule has taken.
5. **Minimum structure (Min-Struct)**: It is the ω with the minimum corresponding PE which a molecule has attained so far.
6. **Minimum potential energy**: When a molecule attains its Min-Struct, Min-PE is the corresponding PE.
7. **Minimum hit number (Min-Hit)**: It is the number of hits when a molecule realizes Min-Struct.

The molecule(s) undergoes one of the following elementary reactions according to the criteria they fall into:

On-wall ineffective collision: Molecule may collide with the container wall and bounce away remaining in one single unit. The transformation of molecular structure is represented as follows: $\omega \rightarrow \omega'$

Decomposition: Molecule may hit a wall, break into smaller parts like ω_1' and ω_2', any mechanism, which can produce $\omega_1'$and $\omega_2'$from ω, is allowed. $\omega \rightarrow \omega_1' + \omega_2'$

Inter-molecular ineffective collision: Multiple molecules may collide and bounce away. The molecularity (assume 2) remains unchanged before and after the process, i.e. $\omega_1 + \omega_2$ and $\omega_1' + \omega_2'$

Synthesis: Synthesis is the opposite of decomposition. Multiple molecules may hit each other and combine, i.e., $\omega_1 + \omega_2 \rightarrow \omega'$. As only one molecule is produced, it is likely to satisfy the energy conservation condition: $PE\,\omega_1 + PE\,\omega_2 + KE\,\omega_1 + KE\,\omega_2 \geq PE\omega'$

2.2 Initializing the major parameters of CRO

Ini-KE: Initial Kinetic energy of the molecule specified by user.
ω: x, y, z values are randomly generated in the range provided.
PE or potential energy: The value of objective function, f (ω).
Pop-size or Population size: Number of molecules undergoing the operations, specified by the user.
Iterations: Number of iterations performed.
Alpha: Probabilistic function for determining unimolecular- collision.
Beta: Probabilistic function for determining inter-molecular collision.
KE loss rate: Decides the rate at which kinetic energy is decreased after collision.
Molecoll: Decides number of molecules involved in collision (1 or more, where b, a randomly generated number decides it).

The parameters of CRO are as defined that are to be initialized using appropriate assumptions. The molecules representing the variables in the given range are generated randomly. Next step defines procedure for selection of random molecule(s), deciding the type of collision by randomly generated parameter (b), and comparing it with predetermined criteria (Molecoll). [6]

Then the selected molecule may undergo any one of the above mentioned reactions. The efficiency of CRO is dependent on these parameters and their values.

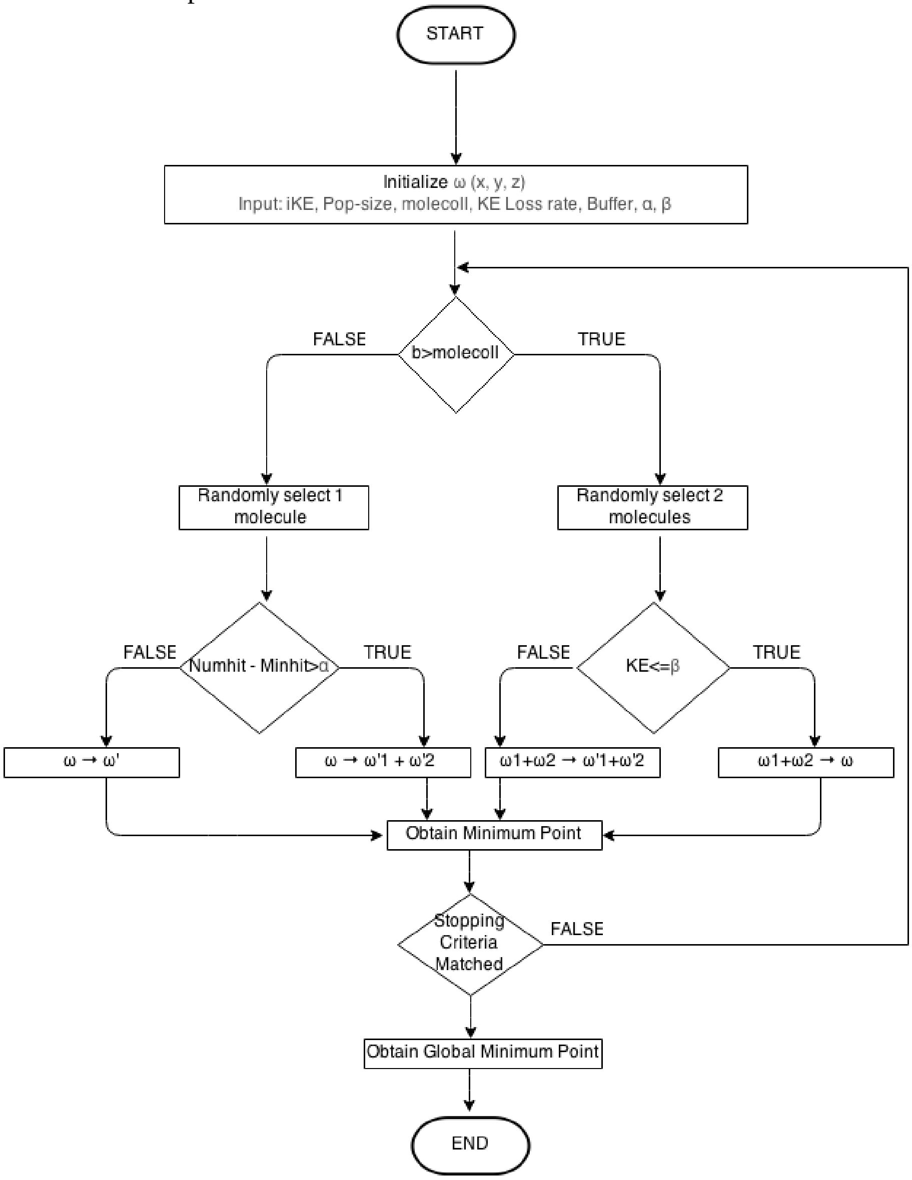

Figure 1: Flowchart for basic algorithm of CRO

IV. RESULTS & DISCUSSIONS

Effect of parameters on optimal solutions obtained using CRO algorithm is studied by conducting numerical experiments. Two non-linear functions containing two and three variables are selected as test functions 1 & 2–. Various test runs are carried by choosing combinations of CRO parameters.

4.1 Test Function 1

Minimize $f(x, y) = (2x-y)^2 + (y+1)^2$

Subject to: $x + y = 10$

CRO was employed to obtain optimal solution for test function 1 and the default values of parameters selected are given in table 1.

Table 1: Default parameter values

Molecoll	Buffer	Ini-KE	KElossrate	α	β	Pop-size
0.2	0	1000	0.2	500	10	100

4.1.1 Numerical experimentations

Various runs have been conducted and table 2, 3, 4, 5, 6 show the variation in test function 1 values obtained for variation in parameters one at a time such as Population size, KE loss rate, Molecoll, Alpha & Beta respectively.

Table 2: Objective function values for variation of Population size

S.No.	Population Size=10	Population Size=100	Population Size=1000	Population Size=10000
1.	54.1091	52.9926	52.9018	52.906
2.	53.828	52.9847	52.9157	52.9055
3.	74.8794	52.9422	52.9077	52.9043
4.	60.2847	52.9746	52.9225	52.9005
5.	53.7375	52.9454	52.9004	52.9013
6.	53.4851	52.9603	52.9127	52.9005
7.	63.4479	52.9155	52.9026	52.9006
8.	54.0415	53.0583	52.9057	52.9014
9.	57.9029	52.9108	52.9358	52.9029
10.	53.8056	53.3874	52.9226	52.9045
Avg:	**57.95217**	**53.00718**	**52.91275**	**52.90275**

Table 3: Objective function values for variation of KE Loss Rate

S.No.	KE Loss rate=0.2	KE Loss rate=0.4	KE Loss rate=0.6	KE Loss rate=0.8	KE Loss rate=1
1.	52.9926	52.9118	52.9777	53.0483	53.0444
2.	52.9847	53.096	53.0198	52.9602	52.9726
3.	52.9422	52.9188	52.9752	52.9096	53.0005
4.	52.9746	52.935	52.9578	52.9675	52.9276
5.	52.9454	52.9648	52.9515	53.0071	53.0866
6.	52.9603	52.9921	53.017	52.9479	53.0298
7.	52.9155	53.0261	53.1451	53.0155	52.9837
8.	53.0583	53.0195	52.9414	52.9361	52.9206
9.	52.9108	52.9529	53.2324	52.9479	53.0133
10.	53.3874	52.9138	52.9589	52.9479	52.9735
Avg:	**53.00718**	**52.97308**	**53.01768**	**52.9688**	**52.99526**

Table 4: Objective function values for variation of Molecoll

S.No.	Molecoll=0.2	Molecoll=0.5	Molecoll=0.8	Molecoll=1
1.	52.9926	52.9728	53.0176	52.9835
2.	52.9847	52.9242	52.9047	53.0273
3.	52.9422	52.9542	52.9656	53.0292
4.	52.9746	52.9316	52.9654	52.9393
5.	52.9454	52.9107	52.9555	52.9169
6.	52.9603	52.9733	52.9584	52.9902
7.	52.9155	52.9546	52.9404	52.9196
8.	53.0583	52.9177	53.0225	52.9765
9.	52.9108	52.9372	52.9606	52.9561
10.	53.3874	52.9659	52.959	53.0318
Avg:	**53.00718**	**52.94422**	**52.96497**	**52.97704**

Table 5: Objective function values for variation of alpha

S.No.	alpha=500	alpha=50	alpha=5
1.	52.9926	53.0185	52.9547
2.	52.9847	52.9647	52.9281
3.	52.9422	52.9715	52.9067
4.	52.9746	53.1501	53.0465
5.	52.9454	52.9411	52.936
6.	52.9603	52.9696	52.9303
7.	52.9155	52.902	52.9048
8.	53.0583	52.9325	52.9287
9.	52.9108	52.9545	52.9932
10.	53.3874	52.9596	52.9651
Avg:	**53.00718**	**52.97641**	**52.94941**

Table 6: Objective function values for variation of Beta

S.No.	beta=10	beta=100	beta=1000
1.	52.9926	52.935	53.0057
2.	52.9847	52.9118	52.9767
3.	52.9422	52.9745	53.0526
4.	52.9746	52.9081	52.9314
5.	52.9454	52.9353	52.9792
6.	52.9603	52.9147	52.9271
7.	52.9155	52.9411	52.9731
8.	53.0583	52.9433	52.9252
9.	52.9108	53.0257	52.9374
10.	53.3874	52.958	52.9531
Avg:	**53.00718**	**52.94475**	**52.96615**

4.1.2 Observations & Results

The study of effect of CRO parameters on test function 1 values obtained has been done by plotting these values as a function of population size, KE loss rate, Molecoll, alpha & beta respectively. The nature of graphs obtained are as shown in figure 2, 3,4,5,6 respectively.

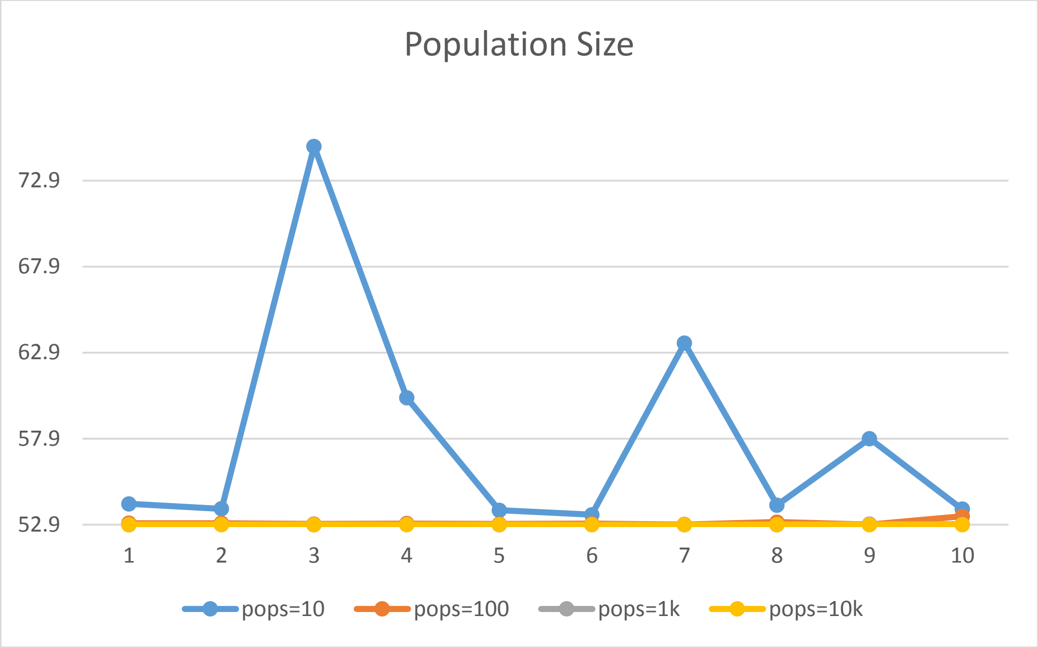

Figure 2: Effect of Population size on test function 1 values

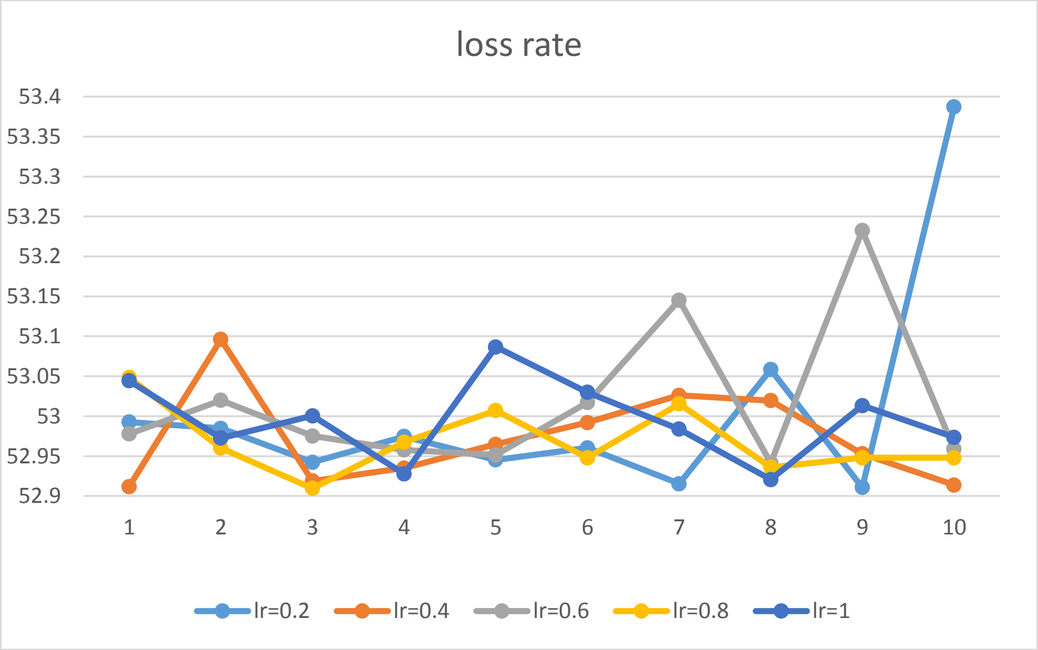

Figure 3: Effect of KE Loss rate on test function 1 values

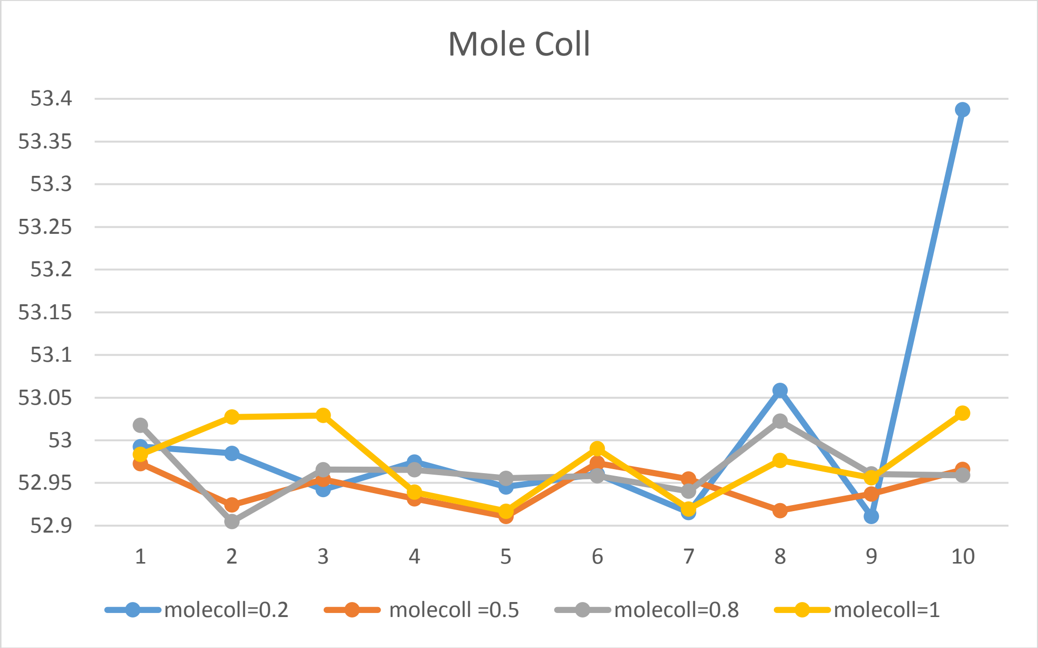

Figure 4: Effect of molecoll on test function 1 values

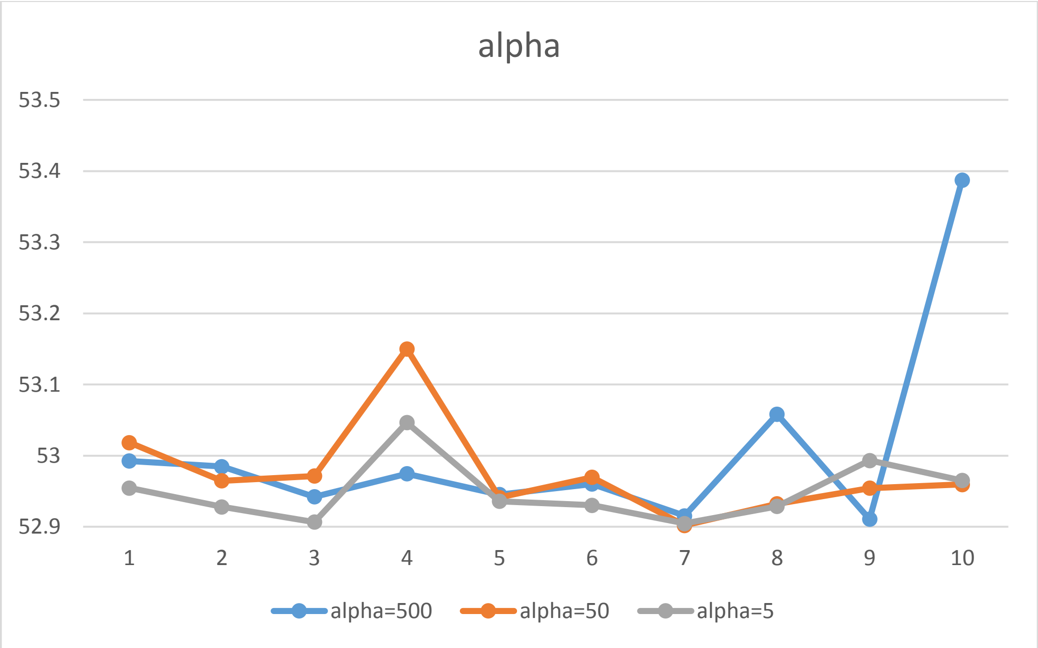

Figure 5: Effect of alpha on test function 1 values

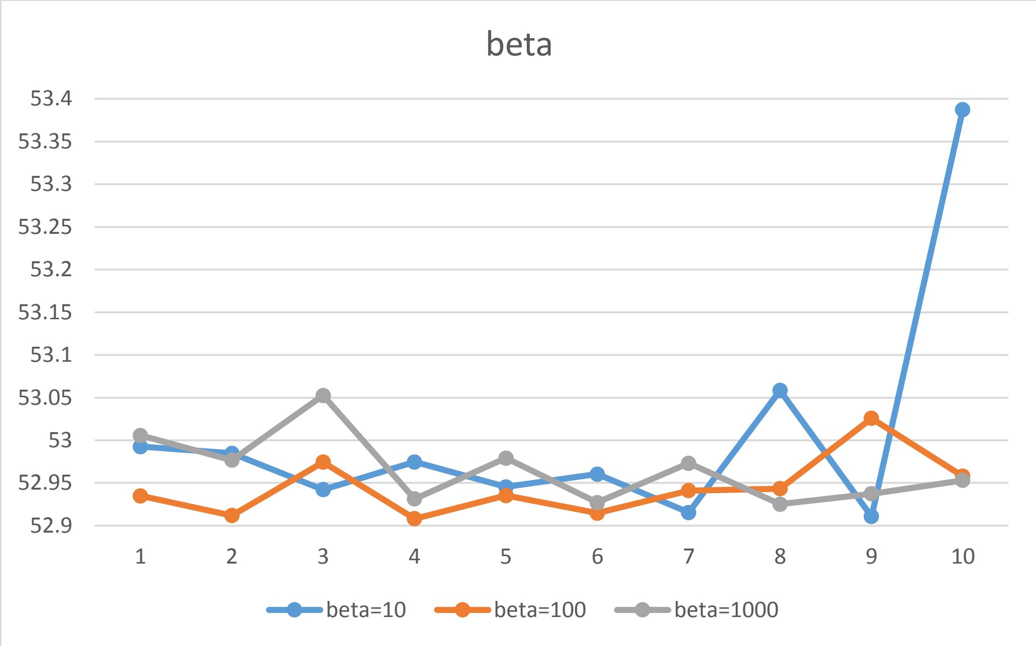

Figure 6: Effect of beta on test function 1 values

As can be seen from these figures the random behavior of CRO is evident for almost all parameters. However following inferences can be drawn:

- The function values become steadier with increase in Population size. The best preferred value of Pop-Size is 10000, based on the average values of function amongst various pop sizes.
- Based on the average values obtained for various runs Molecoll values of 0.5 and 0.8 are observed to give very close best function values.
- Based on the average values obtained for various runs KE loss rate of 0.4 is observed to be the best amongst them.
- Based on the average values of Alpha obtained for various runs Values of alpha=50 and alpha=5 are observed to give very close best function values.
- Based on the average values obtained for various runs value of Beta=100 is observed to be the best amongst them.

4.2 Test Function 2:

Minimize f(x, y, z) = $x^{-2} + 0.25y^2z$
Subject to: $0.75x^2y^{-2} + 0.375yz^{-2} <= 1$
CRO was employed to obtain optimal solution for test function 1 and the default values of parameters selected are given in table 1.

3.2.1 Numerical experimentations

Various runs have been conducted and table 7, 8, ,9 10, 11 show the variation in test function 2 values obtained for variation in parameters one at a time such as Population size, KE loss rate, Molecoll, Alpha, Beta respectively.

Table 7: Objective function values for variation of Population size

S.No.	Population Size=10	Population Size=100	Population Size=1k	Population Size=10k
1.	22.4911	2.9949	1.74675	1.38166
2.	7.86036	3.58463	1.82127	1.31897
3.	3.5865	2.25881	1.3481	1.41671
4.	9.71071	5.6236	1.27871	1.40049
5.	17.8843	1.74858	1.67682	1.32773
6.	7.82097	7.10005	2.1751	1.30263
7.	8.35772	2.27408	2.01214	1.28689

8.	16.23	2.4589	1.72372	1.3298
9.	24.1256	1.47855	1.35589	1.42089
10.	7.96087	4.2703	1.62725	1.27733
Avg:	**12.602813**	**3.37924**	**1.676575**	**1.34631**

Table 8: Objective function values for variation of KE Loss Rate

S.No.	KE Loss rate=0.2	KE Loss rate=0.4	KE Loss rate=0.5	KE Loss rate=0.8	KE Loss rate=1.0
1.	2.9949	1.97404	1.89294	3.62547	2.88708
2.	3.58463	1.90381	2.33757	3.47526	3.21837
3.	2.25881	1.64322	2.52071	2.93709	1.80908
4.	5.6236	1.92379	2.96292	3.31361	4.26966
5.	1.74858	2.05201	3.42373	2.22999	8.1082
6.	7.10005	6.36838	7.90175	2.99251	4.78394
7.	2.27408	1.73916	2.47798	3.21198	1.5776
8.	2.4589	2.80524	2.51387	3.3256	6.43944
9.	1.47855	1.23915	1.57224	4.66798	2.91799
10.	4.2703	2.02094	3.62812	3.62001	2.51069
Avg:	**3.37924**	**2.366974**	**3.123183**	**3.33995**	**3.852205**

Table 9: Objective function values for variation of Molecoll

S.No.	Molecoll=0.2	Molecoll=0.4	Molecoll=0.5	Molecoll=0.8	Molecoll=1
1.	2.9949	2.96192	2.75658	2.65292	3.71179
2.	3.58463	2.32871	2.16404	4.87853	2.27728
3.	2.25881	2.48079	3.73177	1.82031	1.52973
4.	5.6236	4.62186	3.43225	2.07591	2.56659
5.	1.74858	4.12079	2.20795	1.54803	7.56834
6.	7.10005	1.56937	1.88565	4.14505	1.45766
7.	2.27408	4.18155	1.45614	1.80325	2.67859
8.	2.4589	3.42346	4.25819	3.22875	2.72672
9.	1.47855	5.41981	3.25819	2.63032	2.4579
10.	4.2703	4.64788	3.19575	3.05819	2.27409
Avg:	**3.37924**	**3.575614**	**2.834651**	**2.784126**	**2.924869**

Table 10: Objective function values for variation of alpha

S.No.	alpha=500	alpha=50	alpha=5
1.	2.9949	3.26103	2.1098
2.	3.58463	2.91905	1.96418
3.	2.25881	3.61697	2.87849
4.	5.6236	4.11099	2.62055
5.	1.74858	2.68254	7.30972
6.	7.10005	1.97259	2.52619
7.	2.27408	2.51112	3.25129
8.	2.4589	2.42606	3.36689
9.	1.47855	2.55677	2.25743
10.	4.2703	1.68317	2.58929
Avg:	**3.37924**	**2.774029**	**3.087383**

Table 11: Objective function values for variation of Beta

S.No.	beta=10	beta=100	beta=1000
1.	2.9949	2.48965	3.11136
2.	3.58463	3.00282	5.91703
3.	2.25881	2.55803	3.66951
4.	5.6236	1.97858	2.39321
5.	1.74858	1.51319	1.63313
6.	7.10005	3.18807	2.85015
7.	2.27408	2.27356	2.21497
8.	2.4589	2.7628	2.21497
9.	1.47855	3.73309	1.86065
10.	4.2703	3.06922	2.73064
Avg:	**3.37924**	**2.656901**	**2.859562**

4.2.2 Observations & results

The study of effect of CRO parameters on test function 1 values obtained has been done by plotting these values as a function of population size, KE loss rate, Molecoll, alpha & beta respectively. The nature of graphs obtained are as shown in figure 2, 3,4,5,6 respectively.

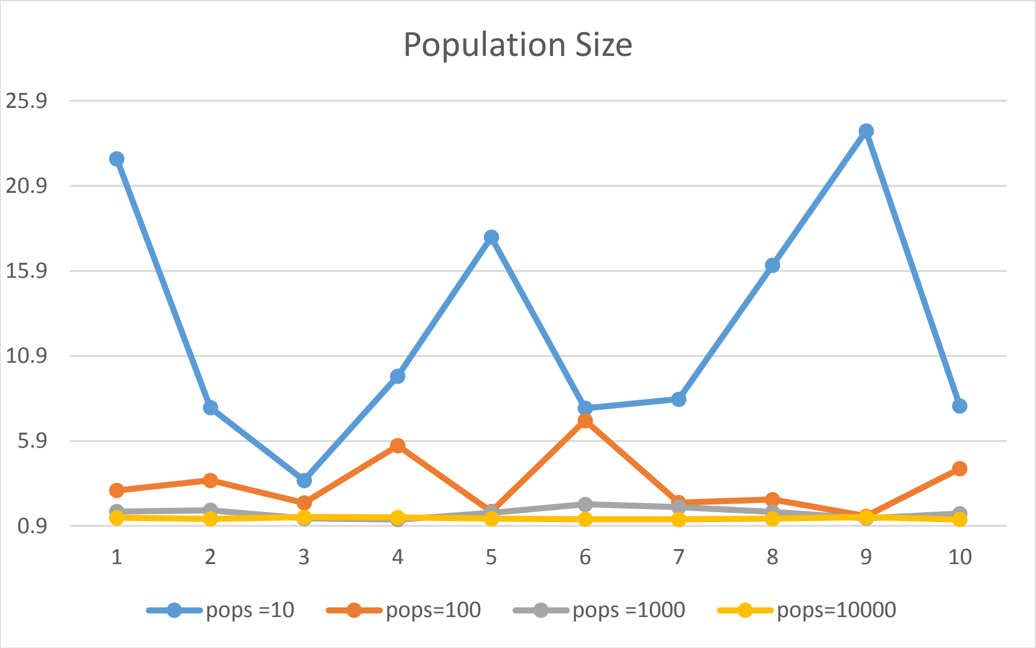

Figure 7: Effect of Population size on test function 2 values

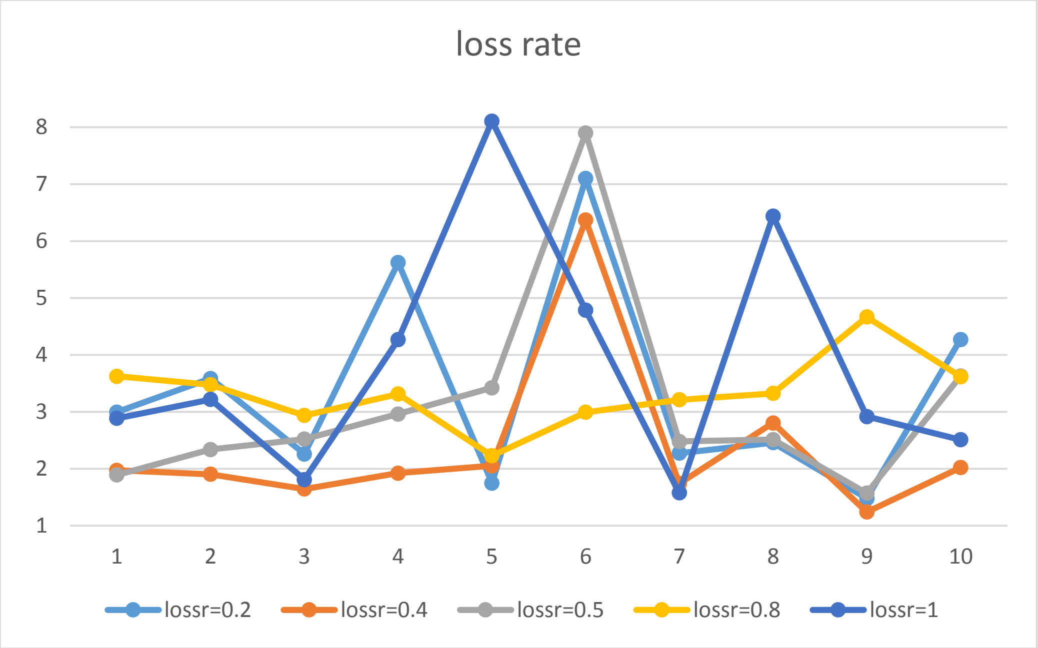

Figure 8: Effect of KE loss rate on test function 2 values

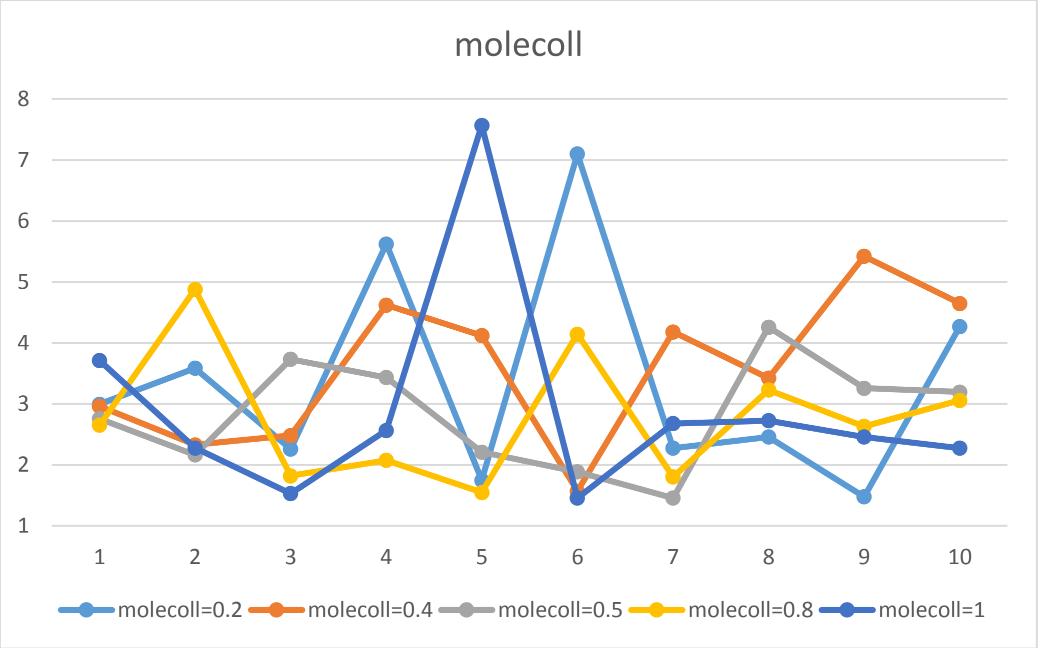

Figure 9: Effect of molecoll on test function 2 values

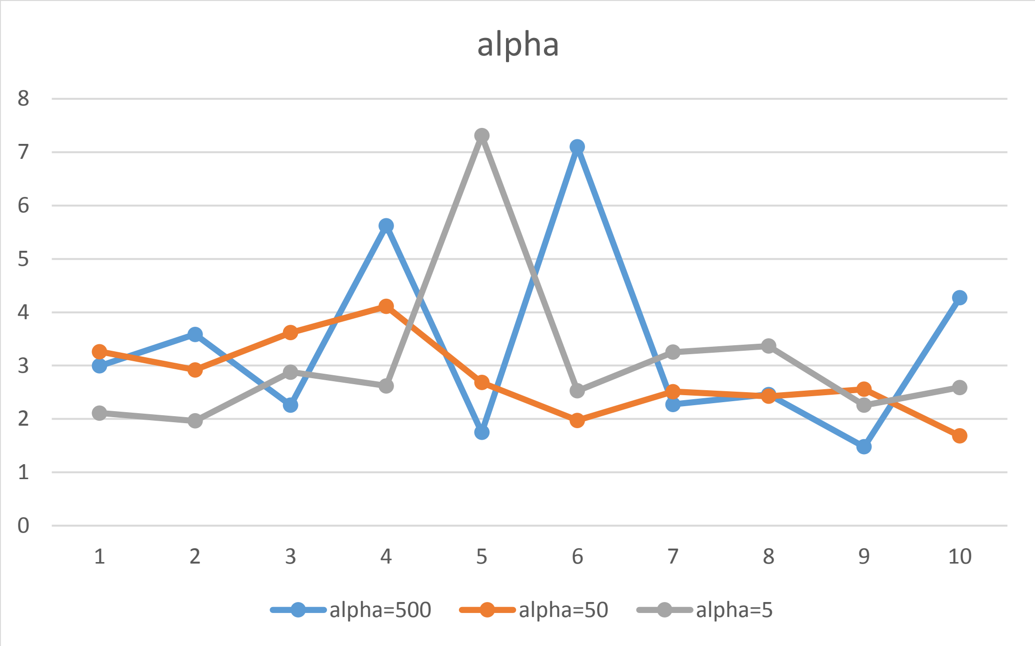

Figure 10: Effect of alpha on test function 2 values

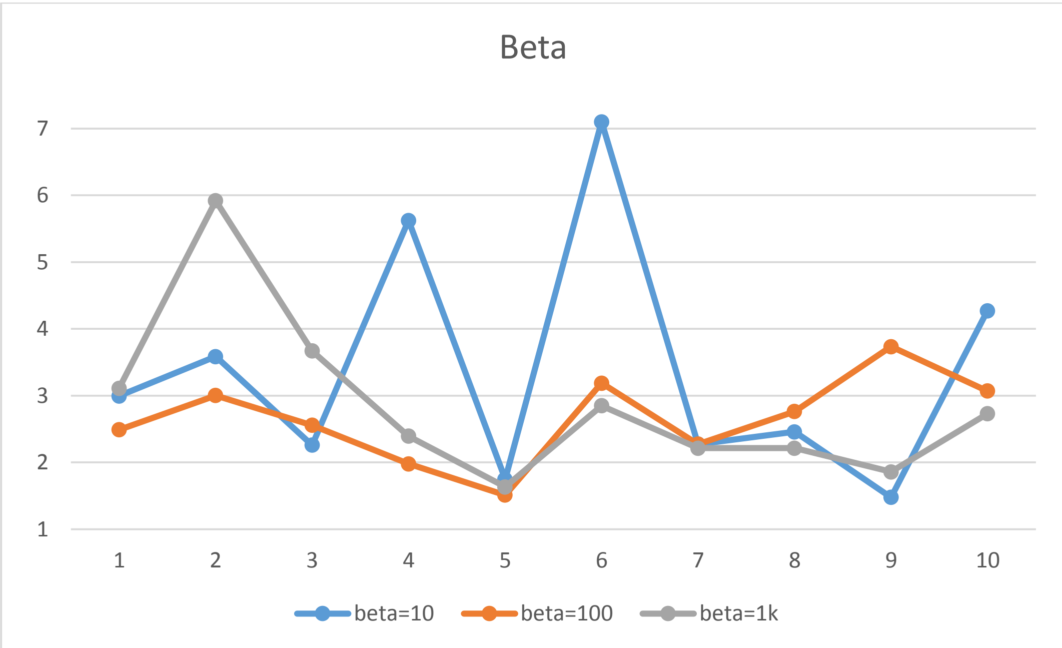

Figure 11: Effect of beta on test function 2 values

As can be seen from these figures, the random behavior of CRO is evident for almost all parameters. However following inferences can be drawn:

- The function values became steadier with increase in Population size. The best preferred value of Pop-Size is 10000, based on the average values of function amongst various population sizes.
- Based on the results obtained from test function 2 the best value for Molecoll, KE loss rate, Alpha & Beta are 0.5, 0.4, 100 and 50 respectively.

4.3 Validation of Optimal Combination of CRO parameters using test function 3

The present work is aimed at arriving at CRO parameters with a right combination of Population size, Molecoll, KE Loss Rate, Alpha and Beta so as to give optimal solutions with lower machine time and randomness. It is also aimed at making the search process more definitive and directed.
Based on the results and discussion of test functions 1 & 2 the optimal combination of CRO parameters suggested are as follows:

Table 12: Suggested Values for parameters

Functions	Molecoll	Buffer	Ini-KE	KElossrate	α	β	Pop-size
Test func-1	0.5/0.8	0	1000	0.4	50/5	100	10000
Test func-2	0.5	0	1000	0.4	50	100	100000
Suggested generic	0.5	0	1000	0.4	50	100	100000

Various runs have been conducted for test functions 1 & 2 using these parameters. The following table shows comparison between the best optimal values obtained using CRO & conventional methods.

Table 13: Comparison of values for test function 1 & 2

	Conventional/Literature Value	CRO Value
Test Function 1	52.9	52.9005
Test Function 2	1.37	1.30263

It can be inferred that CRO is definitely competitive & even superior in obtaining optimal solutions.
The claim is further validated by using these CRO parameters in obtaining solution for test function 3.

Test Function 3:

Minimize $f(x, y, z) = x^{-1}y^{-2}z^{-2}$

Subject to: $x^3+y^2+z<= 1$

CRO parameters values: As mentioned in table 12.
The comparison between the conventional method values/literature values and CRO values obtained of test function 3 using optimal condition is given in table 14.

Table 14: Comparison of values for test function 3

Function	Conventional/Literature Value	CRO Value
Test Function 3	28.36	20.30100

V. CONCLUSION & FUTURE SCOPE

CRO is an emerging natural computing method for optimization, inspired by basic principles of chemical reactions having several advantages over conventional methods that include better speed, more efficiency and ability to target non-linear as well as linear functions. However CRO being a random search method, often leads to lack in the direction while moving towards optimal solution.
The present work is aimed at development of CRO algorithm in C++ & study of effect of its various parameters such as population size, KE loss rate, molecoll, alpha and beta in obtaining optimal solutions so as to make it more definitive & directive in its search. Three non-linear functions involving two or more variables are selected for numerical experimentation. The variation in best optimal function values obtained for various combinations of CRO parameters for two test functions 1 & 2 have been studied thoroughly and optimal combinations of the CRO parameters have been suggested. The validation of these suggested parameter values has been done by employing them to another function, test function 3. The best optimal values obtained using CRO are compared with conventional methods.
Based on the observation and results it can be concluded that CRO has potential of providing optimal solutions with matching or even better performance to conventional methods. Similarly the present work has successfully provided the optimal governing parameters of CRO with improved performance and short machine time and some element of definitive approach in its search in reaching optimal solutions. The work is demonstrative and it is felt necessary that it should be further validated by employing more functions of varied nature.

ACKNOWLEDGEMENT

Authors are thankful to The Director, Laxminarayan Institute of Technology for his constant support & encouragement.

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