MULTI-OBJECTIVE OPTIMIZATION OF BIOETHANOL PRODUCTION PROCESS USING CHAOTIC DIFFERENTIAL EVOLUTION

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Abstract. In process optimization, situations which are multi-objective (MO), where each of the objectives covers different aspects of the problem are encountered with increasing frequency. Therefore, it is critical for the process engineer to have a series of solution choices before selecting of the best solution. In this work, an approach that enhances the differential evolution (DE) algorithm using ideas from chaos theory is introduced. Analysis on the dominance of the solution set produced by these algorithms was carried out using the Hypervolume indicator. This method then was used to generate highly diverse and optimal solutions to the MO bioethanol production process which is a real-world industrial scale problem. Comparative analyses were then carried out with the algorithms developed and employed in this work. Studies on the performance as well as the solution quality produced by these algorithms are presented in this paper.

Keywords: Multi objective (MO) optimization, chaotic differential evolution (CDE), solution measurement, bioethanol production process, hypervolume indicator (HVI).
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INTRODUCTION

In the advent of various cutbacks on fossil fuel sources by global organizations, many industries have made great strides in seeking out potential alternative fuel sources. One of the most feasible and cost effective alternative fuel sources is bioethanol [1]. The existence of significant amounts of sugars such as holocellulose (57–61% by weight) in rice husks makes it a good potential material to be utilized for the production of bioethanol [2]. Efficient ethanol production can be achieved by the reduction of the biomass particle size, maximizing lignin removal, limiting the formation of inhibitors (in the form of degradation products), minimizing the loss of pentose, hexoses and reducing the overall cost of the process [3]. The pre-treatment technique optimized in the work in Banerjee *et al.* [2] is the 'Wet Air Oxidation' technique. This method is a potentially effective pre-treatment technique for fractionating lignocellulose into a solubilized hemicellulose fraction and a solid cellulose rich fraction with minimum inhibitor formation. This then encourages enhanced enzymatic hydrolysis of the material (prior treatment) for the subsequent ethanol fermentation while having minimal inhibitor formation [4], [5]. Thus, the MO optimization of the pre-treatment process of rice husk using the Wet Air Oxidation method to obtain a cellulose-rich substrate amenable to further enzymatic hydrolysis was the main theme of the work by Banerjee *et al.* [2].

In recent times, optimization models and techniques have frequently been used in engineering industries [6], [7], [8], [9]. In MO optimization problems, determining the most efficient solution set can be a very daunting process. In the cases of two objectives, algorithms such as the NSGA-II (Deb *et al*, 2002) have been developed and have proven to be indispensable. For such cases, dominance sorting is possible since only dominant and non-dominant solutions exist. However, in situations involving more than two objectives, the situation is more complicated since there exists various degrees of dominance (such as; strongly dominant, weakly dominant, non-dominant). Due to the difficulty of these sorting and measurement operations such cases, the Hypervolume Indicator (HVI) [10] is employed in this work to quantify the dominance (optimality measure) of the solution sets produced by the algorithm. The Normal Boundary Intersection (NBI) is utilized as a scalarization method in this work to handle the MO nature of the problem [11].

This paper aims to analyze the implementation of the Differential Evolution (DE) [12] and its improved version, the Chaotic Differential Evolution (CDE) techniques for the production of a solution set that dominantly approximates the Pareto frontier in the objective space. These techniques were applied in conjunction with the NBI method to improve the dominance of the solution set during successive iterations. In addition, the level of dominance of the solutions was also measured using HVI performance metric.

This paper is organized as follows: Section 2 presents the Computational Techniques of the while Section 3 gives a brief overview provides the industrial problem formulation. Section 4 describes the dominance measurement approach and Section 5 consists of the analysis of the results and some comparative studies. Finally, this paper ends with some conclusions and recommendations for future work.

COMPUTATIONAL METHODS

Differential Evolution

DE is a type of evolutionary algorithm first introduced by Storn and Price (1995) [12]. The main concept of this technique is the integration of perturbative methods into evolutionary algorithms. DE initializes by the production of a population with a minimum of four individuals denoted as *P*. These individuals are real-coded vectors with a predefined size *N*. The first generation of individual vectors (*gen* = 1) are randomly produced in specific search domains. One principal parent denoted $x^p{}_i$ and three auxiliary parents denoted $x^a{}_i$ is randomly selected from the population, *P*. Every individual, *I* in the population, *P* would become a principle parent, $x^p{}_i$ at one generation or the other. Hence, each individual, *I* have a shot in mating with the auxiliary parents, $x^a{}_i$. The three auxiliary parents then engage in 'differential mutation' to generate a mutated vector, V_i.

$$V_i = x^a{}_1 + F(x^a{}_2 - x^a{}_3) \quad (1)$$

where *F* is the mutation amplification factor such that $x \in R[0,1]$. Next, V_i is then recombined via exponential crossed-over with $x^p{}_i$ to generate child trial vector, $x^{child}{}_i$. The probability of the cross-over, CR is an input parameter set by the user. In DE, the survival selection mechanism into the next generation is called 'knock-out competition' where the principle parent, $x^p{}_i$ is in direct competition with the child trial vector, $x^{child}{}_i$ for the selection of the survivor of the next generation:

$$x_i(gen+1) = \begin{cases} x_i^{child}(gen) \leftrightarrow f(x_i^{child}) \ better \quad than \quad f(x_i^p) \\ x_i^p(gen) \leftrightarrow \quad otherwise \end{cases} \quad (2)$$

The knock-out competition mechanism also serves as the fitness evaluation scheme for the DE algorithm. The parameter setting for the DE algorithm is given in Table 1: The algorithm of the DE method is shown in Algorithm 1.

ALGORITHM 1: Differential Evolution (DE)

Step 1: Initialize individual size *N*, *P*, *CR* and *F*
Step 2:Randomly initialize the population vectors, $x^G{}_{i.}$
Step 3: Randomly select one principal parents, $x^p{}_i$
Step 4: Randomly select three auxilary parents, $x^a{}_i$
Step 5: Perform differential mutation & generate mutated vector, V_i
Step 6: Recombine V_i with $x^p{}_i$ to generate child trial vector, $x^{child}{}_i$
Step 7: Perform 'knock-out' competition for next generation survival selection
Step 8: If the fitness criterion is satisfied and $t = T_{max}$, halt and print solutions
else proceed to step 3

TABLE 1: DE Parameter Settings

Parameters	Values
Individual Size, *N*	6
Population Size, *P*	7
Mutation amplification factor, *F*	0.3
Cross-over Probabbility, *CR*	0.667

Chaotic Differential Evolution

The diversification mechanism used in this work is based on the concept of chaos theory [13]. The idea here is to use chaos-based methods to increase the diversity of the population of solutions produced by the algorithm. In mathematics and physics, chaotic systems are dynamical systems that are deterministic, behave in an irregular manner, highly sensitive to initial conditions and impossible (or difficult) to predict in the long term [14].

In this work, a one-dimensional chaotic map was used to increase the diversity of the population of solutions by embedding the map into the random number generation component in the algorithm. The one-dimensional chaotic map is represented as the following:

$$\psi_{n+1} = f(\psi_n) \quad (19)$$

The most widely studied one-dimensional map is the logistic map [15] which is as the following:

$$f(\psi_n) = r_n \psi_n (1-\psi_n) \quad (20)$$

$$r_{n+1} = r_n + 0.01 \quad (21)$$

where $\psi_n \in [0,1]$ and $r_n \in [0,5]$. In this mapping like all chaotic maps, the dynamics of the system varies for different sets of initial conditions (ψ_o and r_o).

Specific modifications were performed in the DE algorithm to enhance its diversification capabilities by the addition of the chaotic component. First, the population of vectors, x^G_i was generated. The consequence steps are similar to the regular DE algorithm where one principal parent, x^p_i and three auxiliary parents x^a_i are randomly selected. Differential mutation is then performed and the mutated vector, V_i is generated. The V_i is then recombined with x^p_i to generate child trial vector, x^{child}_i. The obtained x^{child}_i is used as the input to the chaotic logistic map. This chaotic logistic mapping is presented as follows:

$$N_i(t) = x_i^{child}(t) \quad (25)$$

$$R_i(t) = \lambda N_i(t) \quad (26)$$

$$N_i(t+1) = R_i(t) N_i(t)\left[1 - N_i(t)\right] \quad (27)$$

$$R_i(t+1) = R_i(t) + \lambda' \quad (28)$$

where $N(t)$ and $R(t)$ are variables in the logistic chaotic map , λ' and λ are relaxation constants specified by the user. Then the logistic mapping is continued until a specific number of iteration is satisfied. The final value at maximum number of iteration of $N(t_{max})$ is incorporated into the child trial vector, x^{child}_i. Hence, the child trial vector, x^{child}_i undergoes another round of mutation by the chaotic map. Next, the 'knock-out' competition for next generation survival selection is performed. The fitness function for the child trial vector, x^{child}_i is evaluated. Thus, another variant of the DE algorithm with enhanced diversification capabilities was developed. In this work, this algorithm is called the Chaotic DE (CDE). The algorithm and the parameter setting are given in Algorithm 2 and Table 2:

ALGORITHM 2: Chaotic Differential Evolution CDE)

Step 1: Initialize population size.
Step 2: Randomly initialize the population vectors, $x^G_{i.}$
Step 3: Randomly select one principal parents, x^p_i
Step 4: Randomly select three auxilary parents, x^a_i
Step 5: Perform differential mutation & generate mutated vector, V_i
Step 6: Recombine V_i with x^p_i to generate child trial vector, x^{child}_i
Step 7: Iterate chaotic logistic map.
Step 8: If $n > N_{max}$, proceed to next step
else go to Step 7.
Step 9: Evaluate fitness of the new $x^{child}_{i.}$
Step 10: If the fitness criterion is satisfied halt and print solutions
else proceed to step 3

TABLE 2: Parameter Settings for the CDE Algorithm

Parameters	Values
Individual Size, N	6
Population Size, P	7
Mutation amplification factor, F	0.15
Max. No. of Evaluations , T_{max}	3000
Constant, λ , λ' , N_{max}	5,0.01, 400

BIOETHANOL PRODUCTION

In Banerjee *et al.* (2009) [2], the data from the experiments were used to build a MO optimization model through multiple regression analysis. This model and the associated constraints are generally presented as follows:

Maximize $\rightarrow$ *Cellulose yield,* f_1
Maximize $\rightarrow$ *Lignin Removal,* f_2
Maximize $\rightarrow$ *Hemicelluloses Solubilisation,* f_3
subject to *process constraints.*

The objective functions (which are Cellulose yield in (%), Lignin Removal in (%) and Hemicelluloses Solubilisation in (%)) as modelled in Banerjee *et al.* (2009) are as the following:

$$f_1 = -38.3467 + 0.6179X_1 + 1.7429X_2 + 3.0846X_3 - 0.0177X_1X_2 - 0.0206X_1X_3 + 0.0937X_2X_3 \quad (6)$$

$$f_2 = -3.8678 + 0.5587X_1 + 18.8545X_2 - 6.9167X_3 - 0.1066X_1X_2 + 0.0347X_1X_3 + 0.0377X_2X_3 \quad (7)$$

$$f_3 = -330.757 + 2.257X_1 - 9.612X_2 + 23.287X_3 + 0.033X_1X_2 - 0.134X_1X_3 + 0.26X_2X_3 \quad (8)$$

where X_1 is the reaction temperature (^oC), X_2 is air pressure (MPa) and X_3 is the reaction time (minutes). The decision variables are constrained as per the experimental setup described in Banerjee *et al.* (2009) .The constraints are as follows:

$$X_1 \in [170,195]$$
$$X_2 \in [0.5,1]$$
$$X_3 \in [10,20] \quad (9)$$

The algorithms used in this work were programmed using the C++ programming language on a personal computer (PC) with an Intel dual core processor running at 2 GHz.

DOMINANCE MEASUREMENT

In this work, the Hypervolume Indicator (HVI) [10] was used to as a dominance measure for the solutions constructing the approximate Pareto frontier. The HVI is a strictly Pareto-compliant indicator that can be used to measure the quality of solution sets in MO optimization problems [16]. Strictly Pareto-compliant is defined such that if there exists two solution sets to a particular MO problem, then the solution set that dominates the other would give a higher indicator value. The HVI measures the volume of the dominated section of the objective space and is highly suitable for multi-dimensional scenarios. When using the HVI, a reference point needs to be specified. Relative to this point, the volume of the space of all dominated solutions can be measured. The HVI of a solution set $x_d \in X$ is formulated as follows:

$$HVI(X) = vol\left(\bigcup_{(x_1,\ldots x_d)\in X} [r_1, x_1] \times \ldots \times [r_d, x_d] \right) \quad (10)$$

where $r_{1,\ldots,}r_d$ is the reference point and $vol(.)$ being the usual Lebesgue measure. In this work the HVI is used to measure the quality of the approximation of the Pareto frontier produced by the DE and the CDE algorithms for various scalar values.

COMPUTATIONAL RESULTS

The approximate Pareto frontiers were obtained using the DE and the CDE techniques. The solutions optimality/dominance was measured using the HVI. For the approximation of the Pareto frontier, 28 solutions for various scalar values were attained for both the algorithms. The approximate Pareto frontiers obtained using the DE and CDE algorithms are shown in Figures 1 and 2 respectively.

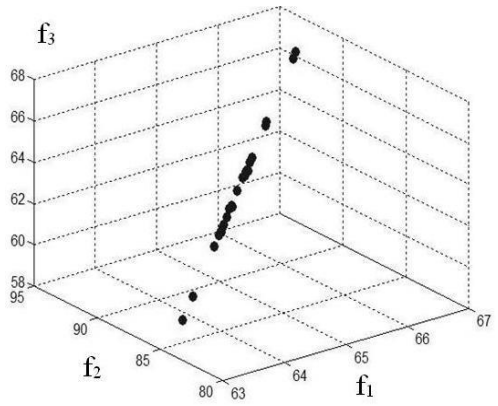

FIGURE 1: Approximate Pareto frontier obtained using the DE algorithm

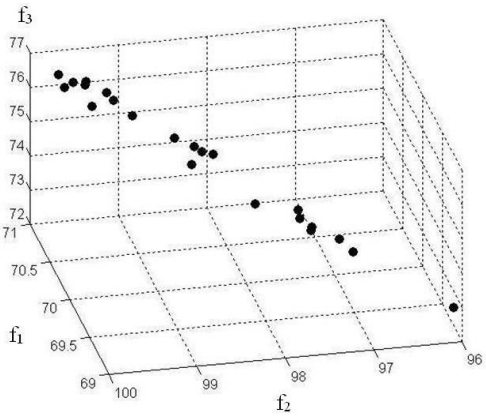

FIGURE 2: Approximate Pareto frontier obtained using the CDE algorithm

Utilizing the HVI, the best individual solution obtained by the CDE algorithm dominates that produced by the DE algorithm by 39.87%. In addition, the DE and the CDE techniques outperformed the solution obtained in Banerjee *et al.* [2]. However, the number of function evaluations taken to obtain the best solution by the DE method is lesser than the CDE method. The comparison of the best candidate solutions obtained by the DE and CDE methods in this work as well as the MINITAB approach in Banerjee *et al.* [2] is shown in Table 3.

TABLE 3: The Comparison of the Best Solutions Obtained By the Techniques

Description		MINITAB [2]	DE	CDE
Objective Function	f_1	66.97	66.414	70.753
	f_2	89	91.083	99.793
	f_3	69.77	67.210	76.872
Decision Variable	x_1	185	181.976	191.93
	x_2	0.5	0.999	0.756
	x_3	15	10.878	10.326
HVI		13084.4	56792.9	79436.6

The best individual solution by DE algorithm was obtained at the scalars w_1=0.4, w_2=0.4 and w_3=0.2. As for the CDE technique, the best individual solution was obtained at the scalars w_1=0.3, w_2=0.3 and w_3=0.4. The HVI computed for the entire frontier of each solution set produced by an algorithm gives the true measure of dominance when compared with any other algorithm. In this work, the HVI for the entire frontier was computed for each of the techniques. The HVI for the entire frontier for the solution sets produced by the MINITAB [8], DE as well as CDE and the associated execution time (in seconds) is shown in Table 4.

TABLE 4: The HVI Obtained By the Algorithms and the Computational Time For The Entire Frontier

	MINITAB [8]	DE	CDE
HVI	-	208012	232293
Comp. time (secs)	-	13.74	33.48

It can be observed from Table 4 that the Pareto frontier approximated by the CDE approach is more dominant by the DE approach by 11.67%. A new optima was achieved by the CDE technique (see Table 3 and 4) since it outperformed the DE and the MINITAB [2] approaches. Thus, it can be said that the CDE method in this work outweighs the overall optimization capabilities of DE and the technique applied in Banerjee [2] (see Table 4). In terms of computational time taken for the algorithm to produce the entire approximate Pareto frontier, the CDE method takes the longest time followed by the DE method respectively. Although the CDE algorithm produces the most dominant frontier, it sacrifices computational efficiency as compared to the DE technique.

In this work, the DE and CDE algorithms performed stable computations during the program executions. All Pareto-efficient solutions produced by the algorithms developed in this work were feasible. In addition, none of the constraints of the decision variables were compromised. Although, the CDE algorithm performs well relative to the DE algorithm used in this work, it can be clearly seen that the execution time is much higher than the DE algorithm. The CDE algorithm is an enhancement of the DE algorithm by incorporating the chaotic component. This in turn endows the CDE algorithm with high diversification capabilities during the search in the objective space. Consequently this results in high computational time as compared with the DE methods.

CONCLUSIONS

The techniques developed in this work produced highly efficient solutions which constructed the approximate Pareto frontier for the Pre-treatment Process Optimization problem. The solution sets obtained by all the methods employed in this work were feasible as no constraints were violated. The CDE algorithm on the other hand produced the approximate Pareto frontier that was more dominant as compared to the conventional DE algorithm by 11.67%.

For future work, the CDE technique may be utilized and tested for a wider range of MO problems with a variety of problems characteristics. Besides, the CDE technique should also be hybridized with other metaheuristics such as Tabu Search [17], Genetic Programming [18] and Swarm-based [17] approaches. Different metrics should also be utilized for measurements (eg: uniformity metric) so that other forms of features of the solution space may be uncovered (for instance; spread uniformity and diversity). These sorts of information would pave the way for a better understanding of MO optimization problems and techniques for solving them.

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