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Development of a Modified Luus-Jaakola Adaptive Random Search Algorithm for Design of Integrated Algal Bioenergy System

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Process systems engineering (PSE) approaches are useful for facilitating the optimal design and operation of industrial plants. This study develops a modified Luus-Jaakola adaptive random search (LJ-ARS) procedure by incorporating some features from the line-up competition algorithm (LCA). The search procedure is conducted using multiple points, and cooperation is exhibited as each point moves toward the next-best point to improve its position. The search space of each point is influenced by its rank, but a lower limit for the space reduction factor is specified to prevent premature convergence. A probabilistic rounding-off procedure is used for integer variables, while the penalty function approach is used for constraint resolution. This modified algorithm is encoded in Microsoft Excel and Visual Basic for Applications and is used to optimize a mixed-integer nonlinear programming model of an integrated algal bioenergy system, while the original LJ-ARS is unable to locate a feasible solution. The model considers six processes: cultivation of the microalgae Chlorella vulgaris, dewatering, cell disruption, pretreatment, oil extraction, and transesterification. The optimal solution, which has been verified using LINGO 14.0, involves microfiltration (for dewatering) and oven drying, but does not utilize any cell disruption process due to high capital cost and energy requirement. This implies that if residual biomass can be sold, it may be more economical to cultivate more algae than to increase the oil yield by means of cell disruption. Furthermore, it is essential to utilize the residual biomass to ensure that the system produces more energy than it consumes. Finally, it is more economical to use residual biomass to supply energy rather than to sell the residual biomass while purchasing electricity.

1. Introduction

Biomass is known as a carbon neutral fuel, because the CO_2 it emits upon combustion is originally fixed from the atmosphere during growth. The technology required for production of microalgal biomass is already sufficient (Chisti, 2007), although exclusive production of biodiesel may be economically infeasible (Pinzon et al., 2014). Razon and Tan (2011) showed that the net energy ratio (energy output divided by energy input) for production of microalgal biofuel could be less than 1, implying that certain processing pathways consume more energy than they produce. Process systems engineering (PSE) techniques are used to model and optimize bioenergy systems such as biomass gasification (Sun et al., 2014). If a process system is represented as a linear model, location of the optimal solution can be guaranteed using standard methods such as the simplex algorithm. However, significant computational difficulties may be encountered in the optimization of nonlinear models (Martelli and Amaldi, 2013).
According to Jenkins (1997), the assumption of constant cost scaling for bioenergy systems cannot be made without exact data. An MINLP model of a biorefinery by Zondervan et al. (2011) considered 72 process options for various stages such as pre-treatment, fermentation processes, separation processes, and fuel blending. Various algorithms for optimization of NLP/MINLPs are currently in use, and metaheuristic or stochastic techniques are one such class of algorithms. One of these techniques is direct search or adaptive random search by Luus and Jaakola (1973). Variations of the original Luus-Jaakola method have been proposed through addition of region collapse and tolerance value parameters (Luus

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and Harapyn, 2003). Poplewski et al. (2011) used variable-specific parameters rather than a fixed space reduction factor. The use of multiple starting points was first proposed by Litinetski and Abramzon (1998). For constraint resolution within the LJ-ARS framework, Luus (1996) demonstrated the efficiency of a quadratic penalty function coupled with a Lagrange multiplier for models containing equality constraints. Another metaheuristic algorithm that resolves constraints using penalty functions is the line-up competition algorithm (LCA), which was shown to take lesser computation time than other evolutionary algorithms when used to optimize NLP models (Yan and Ma, 2001) and MINLP models representing multi-product chemical batch processes (Yan et al., 2004).

Hybrid algorithms have been formulated to combine the strengths of multiple metaheuristics. Adaptive random search may be used as the primary search pattern, or as a subroutine to a different search procedure. Gao et al. (2004) showed that direct search with particle swarm optimization exhibited better speed and accuracy than basic genetic algorithms and simulated annealing procedures. Jeżowski et al. (2005) showed that direct search works better than genetic algorithms for problems with discrete variables, while Liao and Luus (2005) demonstrated that the LJ algorithm is generally faster and more reliable than genetic algorithms. The LJ-ARS has been used in optimization of nonconvex models (Salcedo, 1992) and models with multiple local optima (Jeżowski et al., 2005). In addition to these advantages, the ease of programming the LJ-ARS has led to its frequent use, but there remains room for improvement.

The Luus-Jaakola algorithm adapted for optimization of discrete variables (Luus, 1975) uses a search procedure around a local optimum, but the global discrete optimum may be located elsewhere. The performance of the LJ-ARS is greatly affected by algorithm parameters (Salcedo et al., 1990) as well as by problem class and characteristics (Liao and Luus, 2005). Furthermore, it has been found that metaheuristics do not always succeed in finding the global optimum quickly or consistently for certain models, such as when phase equilibria and thermodynamics are involved (Fernández-Vargas et al., 2013).

The rest of this paper is organized as follows. The formal problem statement is given in the next section, and the development of the modified LJ-ARS based on the original LJ-ARS and LCA is shown. A mixed-integer nonlinear programming model of an integrated algal bioenergy system is formulated, and is optimized using the modified LJ-ARS. Conclusions about the optimal design are presented.

2. Problem Statement

A mixed-integer nonlinear programming (MINLP) model representing an integrated algal bioenergy system may be written according to the following framework:

$$max\ (f) = \Sigma c^T y - \Sigma k^T x^\alpha \tag{1}$$

$$Ax = y \tag{2}$$

$$x \leq Mb \tag{3}$$

$$Qb \leq h \tag{4}$$

Eq(1) is the objective function of maximizing profit, where c represents the unit prices of net flows y, while k and α represent the cost factor and scaling exponents for nonlinear cost functions of process units with capacity x. Material and energy balances are represented in Eq(2) by process matrix A, the coefficients of which may be variables defined by ad hoc equations. Eq(3) uses the big-M constraint to constrain binary variables b, and Eq(4) uses topological matrix Q to limit allowable process system configurations. The model is considered nonlinear because of nonlinear terms in the process matrix and in the capital cost functions. A modified LJ-ARS is developed and used to optimize this model.

3. Development of Modified Algorithm

The original algorithm of Luus and Jaakola (1973) is initiated by generating a number of random points uniformly given the initial random point and search space. The objective function is evaluated for each point that satisfies all constraints. The best objective function so far is recorded, along with its corresponding location, and this is used as the new starting point for the next iteration.

The line-up competition algorithm (LCA) by Yan and Ma (2001) uses families of points to search the space. Points are no longer discarded, as constraints are resolved using the penalty function approach. Each point conducts its own local search, and the best point within each family is retained. The families are ranked, and each family's search space is then adjusted based on its rank. Some features of the LCA are used to develop the modified LJ-ARS as discussed in the remainder of this section.

The modified algorithm is initialized by generating a number of random starting points and evaluating them according to the objective function f. These points are ranked from worst to best. A movement step is performed by having a point of lower rank move towards the point ranked just above it. The magnitude of this movement is proportional to the difference of their objective function evaluations. The search space of each point varies with its rank, in a manner similar to the scheme of Yan and Ma (2001). However, instead of assigning search space multipliers uniformly between 0 to 1, a minimum value is used to prevent premature convergence. A sample iteration of the modified LJ-ARS is shown in Figure 1.

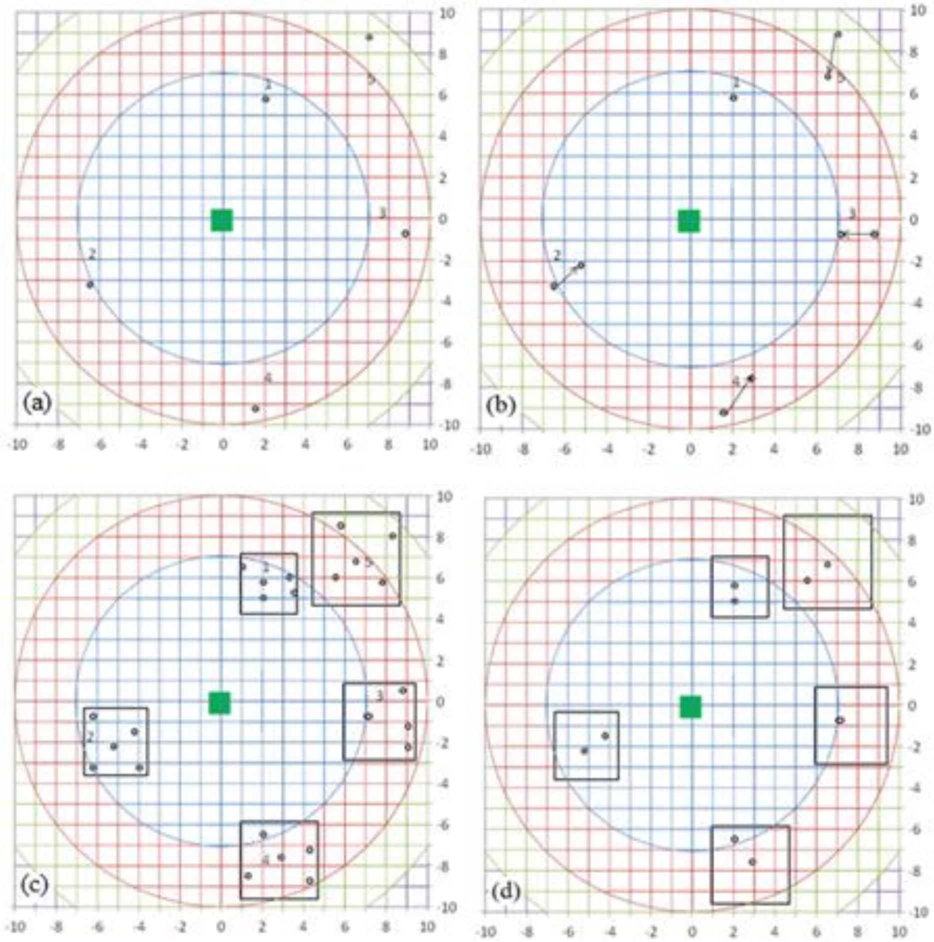

Figure 1: Modified LJ-ARS algorithm for min $f = x_1^2 + x_2^2$: (a) initial generation and ranking, (b) movement, (c) generation of points within rank-based search space, and (d) selection of best point within each family

For discrete variables in MINLPs, the floor and ceiling functions are used to probabilistically round off randomly generated values to the nearest integers. The closer an integer is, the probability that rounding off will be in that direction is increased proportionally. Whenever an unrelaxable constraint is violated, a random feasible location is generated from the nearest allowable value and the current range. However, violations of relaxable constraints are resolved using a penalty function expressed as the weighted sum of constraint violations. The weights are used to give appropriate magnitude against the objective function.

4. Optimal Design of Integrated Algal Bioenergy System

The modified LJ-ARS is used to optimize the MINLP model of an integrated algal bioenergy system containing highly scalable processes within a microalgae-to-biodiesel conversion system (Halim et al., 2012a). *Chlorella vulgaris* with an assumed elemental composition of $C_{106}H_{181}O_{45}N_{16}P$ is cultivated in a raceway pond (Rogers et al., 2014) using wastewater containing nitrogen and phosphorus nutrients. Dewatering to a concentration of 200 kg/m^3 is conducted using either centrifugation or microfiltration. Cell disruption (bead milling or high-pressure homogenization) may be used to increase oil yield. Solar drying has negligible energy requirement compared to oven drying, but it has a higher capital cost. Algal oil is extracted using completely recoverable hexane, and is transesterified into biodiesel. Unit prices of raw materials and products are taken from Yan et al. (2014). Nonlinear cost-capacity functions for the raceway pond are from Chisti (2007), those for the centrifuge, microfilter and bead mill are derived from Loh et al. (2002), and those for the remainder of the process units are from Peters and Timmerhaus (1991). Capacities are expressed in terms of mass flow rate of dry biomass. Table 1 shows the process data used within the model, which contains 28 variables (8 binary and 20 continuous) and 28 constraints. The model and algorithms have been encoded in Microsoft Excel and Visual Basic for Applications (VBA).

Table 1: Process data

Process Unit	Cost-capacity Function ($)	Energy Requirement (MJ/kg dry biomass)	Other Information	References
Raceway Pond	$51,200x^{0.6}$	5.63×10^{-5}		
Centrifuge	$59,500x^{0.49}$	2.15	95 % recovery	Safi et al., 2014
Microfilter	$412,000x^{0.68}$	0.685	100 % recovery	Danquah et al., 2009
Bead Mill	$364,000x^{0.74}$	23.1	96 % algal oil increase	Doucha and Livansky, 2008; Halim et al., 2012b
High-Pressure Homogenizer	$2,740x^{0.6}$	529	405 % algal oil increase	
Oven Dryer	$331x^{0.42}$	7.53 MJ/kg H_2O evaporated	6.4 % less algal oil per 10 % increase in moisture	Genskow et al., 2008
Solar Dryer	$3,540x^{0.6}$	0		
Extraction Vessel	$153x^{0.42}$	2.462		Dassey et al., 2014
Transesterification	$4840x^{0.54}$			

	Unit Cost ($/kg)	Calorific Value	Other Information	References
Biodiesel	1.18	37.0 MJ/kg	Demand of 10,000 t/y	Razon and Tan, 2011
Glycerol	1.03			
Residual Biomass	0.294	9.36 MJ/kg		McKendry, 2002
Electricity	0.0417/MJ			
Methanol	0.557			

The original LJ-ARS failed to yield a feasible solution after 500,000 function evaluations, while the modified LJ-ARS located the following solution in less than 100,000 function evaluations. The system configuration resulting in the maximum annual profit utilizes the following process units: centrifugation for dewatering, no cell disruption process, and solar drying. The optimized system has an overall annual profit of 52.5 M$ and produces biodiesel at a rate of 0.347 kg/s (10,000 t/y for a plant operating 8000 h/y), which is equivalent to 12.8 MW of energy. Some of the residual biomass is used to generate the 25.2 MW of energy required by the process system, while the remainder is sold. The corresponding net energy ratio of this system is 3.36. The solution in Figure 2 has been verified using LINGO 14.0. Gray boxes for process units indicate that they are excluded from the optimal design.

Microfiltration is selected over centrifugation for dewatering, despite its higher capital cost. This may be because of its higher yield and lower energy requirement. Neither of the cell disruption processes is used within the optimal configuration. The capital cost of a bead mill is too high, while the energy requirement of the high-pressure homogenizer is not justified by the increased yield of algal oil. Oven drying is used despite the energy requirement, but its capital cost is lower than that of solar drying. The mass flow rate of the dry biomass remains constant throughout dewatering and pretreatment.

The optimal solution settles for a low yield of algal oil from dried biomass, choosing instead to produce a larger mass of algae and discard most of it as residual biomass. This implies that it may sometimes be more economical and energy-efficient to cultivate more algae rather than disrupt algal cells to increase their oil yield upon extraction. This may hold true because the wastewater fed to the raceway pond has no associated purchasing costs. All the electricity requirements are supplied by the residual biomass, implying that it is more economical to use residual biomass as fuel rather than to sell it while purchasing electricity. Cultivating a large amount of algae corresponds to a large amount of residual biomass after oil extraction, and the sale of all the residual biomass can improve the economic feasibility of the system. The solution also reveals that residual biomass may contribute more profit and energy to the system compared to biodiesel, and the net energy ratio of the system would be less than 1 if the only equivalent energy considered is that of biodiesel. This implies that utilizing residual biomass is necessary for the system to be feasible in terms of energy generation.

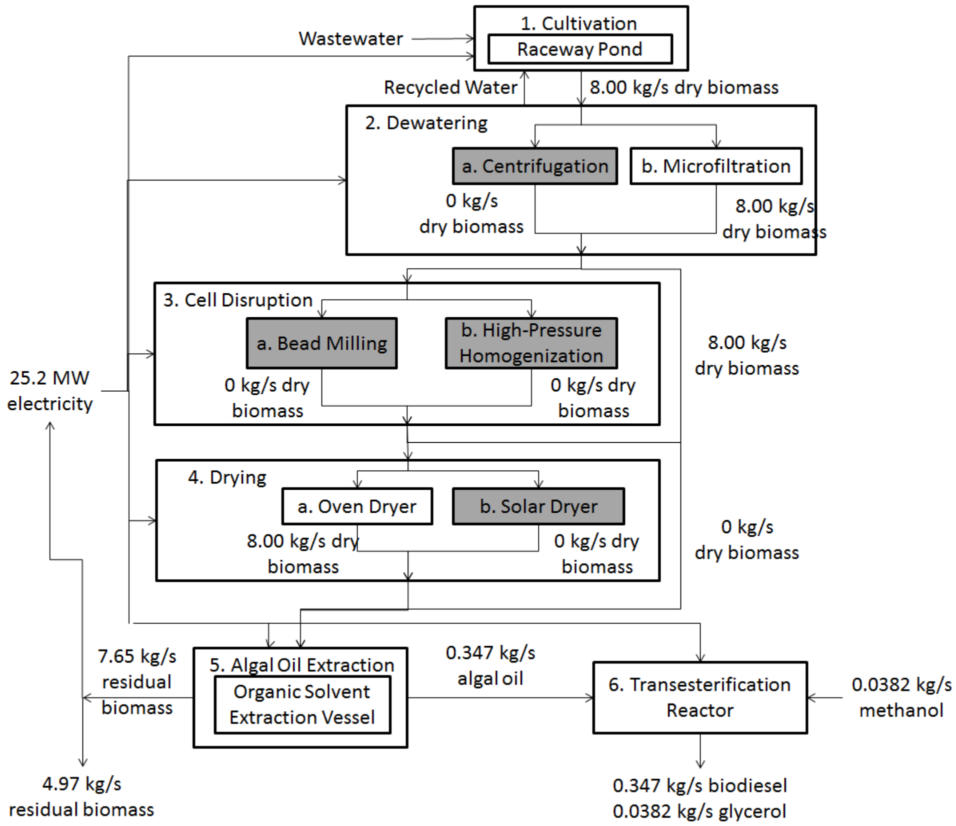

Figure 2: Flowchart of Optimal Integrated Algal Bioenergy System

5. Conclusions

A modified Luus-Jaakola adaptive random search (LJ-ARS) algorithm has been developed by incorporating features from the line-up competition algorithm (LCA). This modified LJ-ARS locates the optimum of the integrated algal bioenergy system model, while the original LJ-ARS is unable to find a feasible point. The final solution obtained indicates the maximum annual profit and the corresponding net energy ratio. It also reveals the optimal configuration and capacities of the process units, as well as the resulting net flow rates of raw materials and products. The solution demonstrates that the capital costs and energy requirements of cell disruption may be too high to justify the higher yield of algal oil extraction. Utilizing some of the residual biomass as fuel for the system can be less costly than purchasing electricity, and sale of any remaining biomass further improves the profitability of the system. Future work may include the modelling of additional process alternatives, manufacture of high-value chemical products, or may address uncertainties in the model, such as in the process data.

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