

Application of a genetic simulated annealing algorithm for data reconciliation

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Abstract

To elucidate the propagation of error or bias from the measurement of a process, the data requires reconciliation. In this article, a genetic simulated annealing algorithm (GSA) based program is proposed for solving data reconciliation (DR) problems. The proposed GSA utilizes simultaneous simulated annealing and modified cross-generational probabilistic survival selection (CPSS) in a genetic algorithm. Validation is performed with linear and nonlinear DR problems. The test starts with the study of appropriate GSA parameters of constraint problems. The performance of GSA with the appropriate parameters is then compared to the genetic algorithm (GA) method, the specific method, and the commercial software DATACON. The proposed GSA, with its ability to give more accurate reconciled data, is a promising choice as an optimization tool for data reconciliation problems.

Key words

data reconciliation, genetic simulated annealing algorithm, optimization

1. Introduction

Data on the real state of physical variables and processes can be obtained from measurements; these, however, are only estimates. Process data measurements are generally corrupted with two types of errors—random and gross—causing violation of process constraints defined by the

mass and energy balances [1]. Therefore, the elimination of such errors would improve the accuracy of measured data. Data reconciliation adjusts process measurements with random errors by supplying satisfactory material and energy balance constraints. Elimination of the

less frequent gross errors, which can severely bias the estimates and the reconciled data, is achieved by gross error detection.

Therefore, simultaneous data reconciliation and gross error detection have emerged [2]. In chemical engineering, Kuehn and Davidson [3] proposed the first solution to the steady-state data reconciliation problem. Later, Crowe et al. [4] investigated measured and unmeasured variable linear systems using matrix projection. A solution of the nonlinear data reconciliation problem via successive linearization is described by Knepper and Gorman [5]. Tjoa and Biegler [6] proposed an efficient hybrid successive quadratic programming algorithm to solve the bi-variable objective function of DR problems. Sánchez and Romagnoli [7] applied Q-R factorization to analyze, decompose and solve linear and bilinear reconciliation problems. To avoid complex calculations resulting in a complicated process, Zhao and Jiang [8] proposed a stochastic search method for solving the linear steady-state DR problem. The significant advantage of this method is that it does not depend on any particular model structure and only requires simple algebraic calculation.

A popular stochastic search, genetic algorithm (GA), is widely used to solve optimization problems. Wongrat [9] developed GA for the DR problem defined by a redescending estimator and weighted least squares. This GA can solve the

DR problem without the complex calculations required by conventional optimization methods, but the calculation time is longer and the data result is not satisfactory for complex systems. GA provides a solution to the complicated problem of discontinuous and non-convex objective functions determined without using derivatives. A notable characteristic of GA is that it can find the region of optimal values rapidly; however, the ability to accurately search in this region is not satisfactory for complex systems [10].

For this reason, many researchers have tried to design new hybrid algorithms by combining GA with other optimization algorithms. Simulated annealing (SA) is an approach for simulating the thermodynamic process of annealing (cooling of a solid). It has been observed that this method could also be used to search for feasible solutions of optimization problems with the objective of converging to an optimal solution. SA can search accurately in certain regions; however, it is difficult to explore the entire search space. Therefore, the difficulty of solving complex problems can be overcome by improving GA by combining it effectively with an SA algorithm to avoid the common defect of early convergence. This is known as a genetic simulated annealing algorithm (GSA).

GSA will be proposed in this article as the best method for handling the discontinuous and non-convex properties of objective function

in steady-state DR problems. In the following section we describe the general formulation and objective function for DR. In Sections 3 and 4, the basic theory and procedure of using GSA for DR will be discussed. In section 5. DR problems are solved with GSA and also compared with other methods.

2. General formulation of the data reconciliation problem

The estimation of unmeasured variables, and model parameters, are obtained as part of the reconciliation problem. The estimation of unmeasured values based on the reconciled measured values is also known as data coaptation. In general form of data reconciliation problems.

$$\begin{aligned}
 & \min_{x,u} \rho(x^M, x) \\
 & h(x, u) = 0 \\
 & g(x, u) \leq 0 \\
 & x^L \leq x \leq x^U \\
 & u^L \leq u \leq u^U
 \end{aligned} \tag{1}$$

where: ρ is an objective function depending on the difference between the measurement of a variable and its value for any measured variables; EMBED Equation.3 is the set of measurement data of the corresponding variable x ; u is the set of unmeasured variables; h is the set of equality constraints; g is the set of inequalities; and superscripts L and U are the lower and upper bounds of the variables.

The objective function usually uses a weighted least squares objective function. However if there are gross errors in the data, the objective function is biased, leading to incorrect data reconciliation. The common procedure is to identify and eliminate gross errors. Thus data reconciliation and gross error detection are applied together to improve the accuracy of measured data. This paper uses weighted least squares and a redescending estimator as objective functions – the weighted least squares method is used for data reconciliation problems, and a redescending estimator [11] for data reconciliation of measured data containing gross errors.

Objective Function for data reconciliation

We discuss the form of M-estimators for the objective function EMBED Equation.3 in Eq. (1). The M-estimators are defined as:

Least squares estimator

$$2C_F^2 \left[\frac{|\varepsilon_i|}{C_F} - \ln \left(1 + \frac{|\varepsilon_i|}{C_F} \right) \right] \tag{2}$$

where $C_F = 1.3998$

Hampel's redescending M-estimator

$$\begin{aligned}
 & \frac{1}{2} \varepsilon_i^2, & 0 \leq |\varepsilon_i| \leq a \\
 & a|\varepsilon_i| - \frac{1}{2} a^2, & a < |\varepsilon_i| \leq b \\
 & ab - \frac{a^2}{2} + (c-b)\frac{a^2}{2} \left[1 - \left(\frac{c-|\varepsilon_i|}{c-b} \right)^2 \right], & b < |\varepsilon_i| \leq c \\
 & ab - \frac{a^2}{2} + (c-b)\frac{a}{2}, & |\varepsilon_i| > c
 \end{aligned} \tag{3}$$

where $c \geq b + 2a$

The consequence of this tuning requirement is that in data reconciliation and gross error detection, the performance of two different EMBED Equation.3 functions can be compared properly only for (nearly) equal efficiency cases.

This means that, for instance, Fair function Eq.(2) with 95% efficiency can be compared with 95% efficient Hampel's redescending M-estimator in Eq.(3) and the value of QUOTE and c are 1.35, 2.7 and 5.4.

3. Genetic Simulated Annealing (GSA) Algorithm

In normal GA, only simple crossover, mutation and selection are used as the genetic operators; normal GA cannot embody a complicated evolutionary process. Because of the limitation of population size and number of generations, the algorithm can easily produce truncation error, which will lead to precocity. For this reason, many researchers have attempted to design new hybrid algorithms by combining GA with other optimization algorithms. All of these hybrid algorithms are able to improve the efficiency of GA to a certain degree.

SA is a powerful optimization technique which can theoretically converge asymptotically to the global optimum solution with probability '1' when the initial temperature is high enough and the temperature decrease is infinitely slow.

The process of this evolutionary operation adopts the new values based on the Boltzmann rule.

$$\exp\left(\frac{-\Delta E}{kT}\right) \geq \text{random}(0, 1) \quad (4)$$

This rule is expressed in the following form: Here, EMBED Equation.3 is the difference of fitness value between the child generation and the parent generation, and T is the annealing temperature. The main drawback of SA in practice is that the parameters in SA are hard to control. Firstly, there is a contradiction between optimization efficiency and computation time in the selection of the annealing rate. If the cooling rate is excessively fast, the evolutionary operation may miss the extremity. However, the convergence rate of this algorithm will be very slow. Secondly, for every temperature, SA by itself cannot easily determine if it has reached the balanced state. This means the length of the Markov chain cannot be controlled easily. Moreover, when it is reflected to the algorithm, the timing of the Metropolis process is difficult to control. Selection of the initial temperature is another difficulty in the application of SA [10].

A simple integration method for GSA algorithms is to generate new individuals with GA; then these individuals are processed with SA, and the results are used as the initial individuals of the next generation.

4. Methodology

Procedure of Genetic Simulated Annealing Algorithm for data reconciliation

Selected data reconciliation problems have two kinds of variables: measured and unmeasured. But data reconciliation problems are only concerned with measured variables. Thus we need to eliminate unmeasured variables from the constraint equations. Since the unmeasured variables are present in the equations, the simplest strategy for solving the problem is to eliminate them from the constraints. This will not affect the objective function since it does not involve unmeasured variables. After that the reconciled values of unmeasured variables can be calculated using the original constraints. Thus, GSA will act as a tool for searching the solution space for only measured variables. Usually GSA can randomly produce solutions that satisfy equality constraints. GSA has also been used to solve constrained optimization problems. Although different methods for handling constraints have been suggested, penalty function methods have been most widely used. The GSA procedure for data reconciliation used in this work follows the steps below and show in the Fig. 1:

Step 1 Choose real coding to represent problem parameters and roulette wheel selection methods, intermediate recombination, and real value mutation. Typically a binary representation is used in GA, but this has disadvantages when

applied to multidimensional high-precision numerical problems. In these cases, the binary GA becomes inefficient and solutions require a large number of computational operations. Real number representation can deal with this problem and is more understandable than binary representation.

Step 2 Assign appropriate GSA parameters consisting of:

- Mutation probability, P_m . Mutation operates on an individual (chromosome), producing offspring very different from the parent. Certain genes in the offspring chromosome are randomly altered with a mutation rate, P_m . P_m controls the rate at which new genes are introduced into the population. A low rate will prevent the introduction of potential genes, while a high rate will allow too much random perturbation. Mutations encourage a population that is converging onto some optimum to jump into a different part of the solution space, thus increasing the probability of detecting a different point leading to the global optimum solution. In this paper, multi-position mutation is used for the mutation operator.

- Crossover probability, P_c . Crossover is used to create two new chromosomes from two existing chromosomes selected from the current population using a crossover rate (PC). The crossover rate is defined as the ratio of the number of offspring produced in each population size.

This ratio controls the expected number of chromosomes which undergo the crossover operation. A higher crossover rate allows more exploration of the solution space and reduces the probability of a local optimum. However if this rate is too high, unnecessary computational time will be consumed in exploring unpromising regions of the solution space. For real number representation, crossover is determined by using a linear combination of two vectors, termed arithmetic crossover.

- Population size, N
- Generation number, g
- Decrease in temperature, α
- Initial temperature, T₀
- Final temperature, T_f
- Annealing function

One way to decrement the temperature is a simple linear method. An alternative is a geometric decrement where , where $t = t\alpha$, where $\alpha < 1$.

From other research has shown that α should be between 0.8 and 0.99, with better results being found in the higher end of the range. Of course, the higher the value of α , the longer it will take to decrement the temperature to the stopping criterion.

And the annealing function is the function to generate new points for the next iteration. The choices are “annealingfast” and “annealingboltz”

- annealingfast : The step has length temperature, with direction uniformly at random. This is the default.

- annealingboltz : The step has length square root of temperature, with direction uniformly at random.

Step 3 Set generation number g=0, temperature T=T₀.

Step 4 Find initial solution P(g) to population size N.

Step 5 If g > gmax, terminate.

Step 6 Evaluate each chromosome of P(g) from the objective function and evaluate the fitness function, which is normally used to transform the objective function value into a measure of relative fitness, while the selection algorithm selects populations for reproduction on the basis of their relative fitness. The selection process is used to choose chromosomes from the parent and the offspring to make up a new population with the same number as the existing population. Wasanapradit [13] adopted CPSS (cross-generational probabilistic survival selection) as the selection method.

Step 7 Perform reproduction on the population, crossover on random pairs of strings, and mutation on every string.

Step 8 Calculate energy (E) using the equation:

$$E = E(x^{(g+1)}) - E(x^{(g)}) \quad (5)$$

where : $E(x^{(g+1)})$ = objective function value of new string

$E(x^{(g)})$ = objective function value of old string

If E is negative, then the new string is better than the old one, and is accepted for the next generation, if not recalculate in Step 1.

Step 9 Calculate the acceptance probability using the acceptance algorithm:

$$Pr_E = \exp(-E/T(g)). \quad (6)$$

- Generate a random number (r) between (0, 1).
- If $r \leq Pr_E$, accept new (child) chromosome in a new generation; if not, use the old (parent) chromosome.

Step 10 Evaluate strings in the new population. Set $g = g+1$, then lower T according to the schedule and go to Step 6.

5. Results and Discussion

5.1 Case study

In this paper, weighted least squares and a redescending estimator are used as the objective functions for data reconciliation problems. Both objective functions and constraint equations require very complex calculations for data reconciliation EMBED Visio.Drawing.11

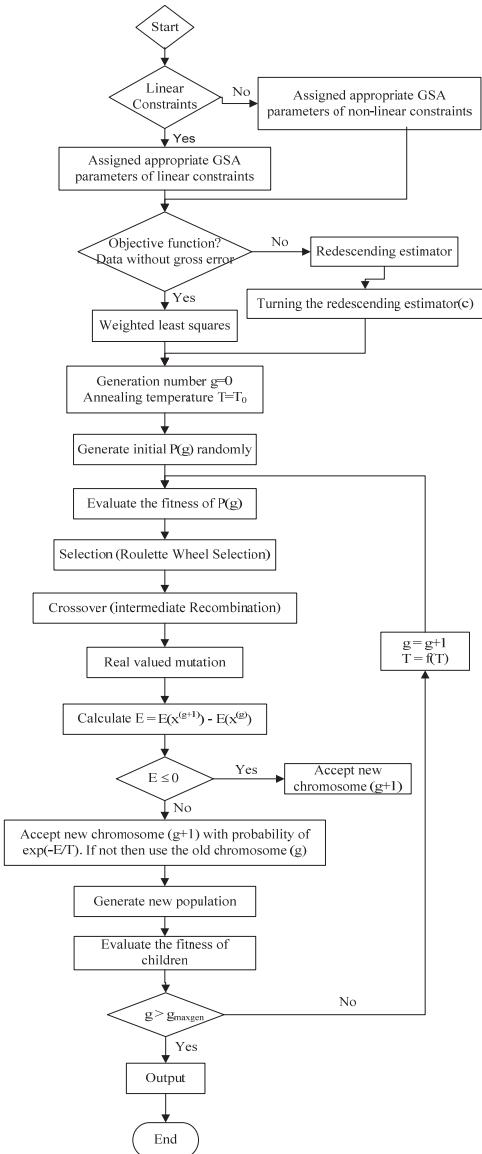
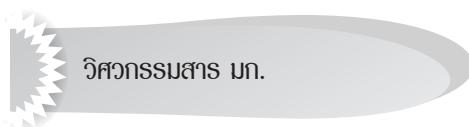


Fig. 1. Genetic simulated annealing algorithm (GSA).

using conventional optimization methods. Therefore, a genetic simulated annealing algorithm (GSA) is proposed as an optimization tool for data reconciliation problems in this work. We perform the GSA based on a typical weighted least squares objective function for simple data reconciliation



problems where the measured data contain only random errors. (The objective function for data reconciliation problems in which the measured data contain random errors and gross errors is important because it can eliminate combinatorial procedure for gross error detection and use straightforward methods to identify them.) Moreover, gross error detection using statistical tests based on linear or linearized models is not suitable for nonlinear data reconciliation problems. The proposed code for data reconciliation problems is developed using MATLABTM. All examples have been solved using a computer with an AMD AthlonTM XP 2000+ 1.67 GHz microprocessor and 256 MB of RAM.

5.2 Appropriate GSA parameters

This section will investigate and select the appropriate parameters for GA and SA, which are considered in two cases as linear and nonlinear constraint problems (Tables 1). These

parameters will be employed in the following case studies

As one can see in Fig.2 (a) and 2(c), we select the value of P_c that has a least scatter of P_m for linear constraint and nonlinear constraint (0.2 and 0.9). In the same way, in Fig. 2(b) and 2(d) the P_m at 0.9 and 0.3 is selected. We also find that the calculation time has no significant. The objective function value is 1.3619 and 0.06646.

Table 1. GSA parameters for problems

| Parameter | Linear | Nonlinear |
|-----------------------------------|---------------------|---------------------|
| | constraint Value | constraint Value |
| Mutation probability, P_m | 0.9 | 0.3 |
| Crossover probability, P_c | 0.2 | 0.9 |
| Population size, N | 40 | 40 |
| Generation number, g | 5000 | 5000 |
| Decrease in temperature, α | 0.99 | 0.99 |
| Initial temperature, T_0 | 10000 | 10000 |
| Final temperature, T_f | 1.00E-02 | 1.00E-02 |

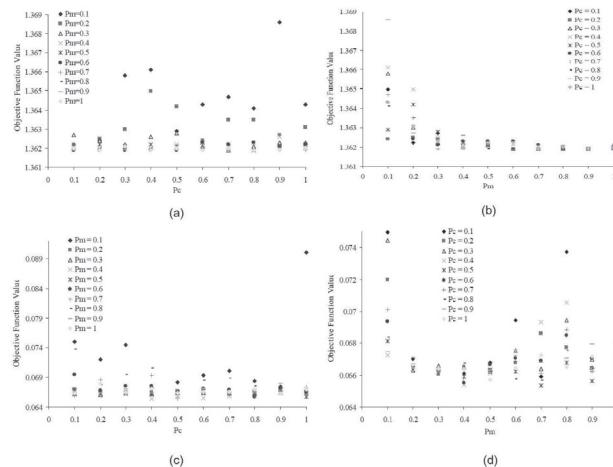


Fig. 2. The objective function value of problems: (a) linear constraint problem at fixed P_c and variances P_m (b) linear constraint problem at fixed P_m and variances P_c (c) nonlinear constraint problem at fixed P_c and variances P_m (d) nonlinear constraint problem at fixed P_m and variances P_c .

5.3 Simple linear data reconciliation

This problem is used to illustrate a number of basic features of data reconciliation. Fig. 3 shows four units with eight stream processes designed to perform a reconciliation of the mass flows.

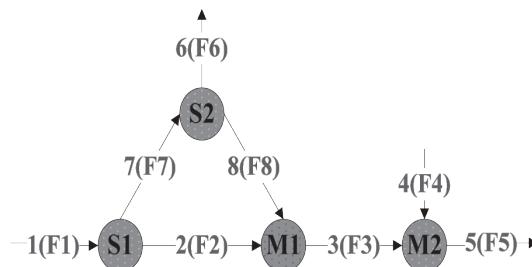


Fig. 3. Mass balance problem.

Let us assume that streams 7 and 8 are unmeasured, streams 1 and 3 are measured with

a standard error of 1%, streams 2, 5 and 6 are measured with an error of 2%, and stream 4 is only approximately measured with a 5% error (Table 2).

The appropriate GSA parameters used in this case were formulated with linear constraints, and with weighted least squares as the objective function. A comparison of the performance of GA, DATACON and GSA is shown in Table 2.

The proposed GSA technique gives the best objective function value (1.3619), which is very close to the DATACON result. Therefore, the SA can support the GA and provide a significant search advantage. In addition, all three approaches have reconciled the data and calculated the values of streams 7 and 8.

Table 2. Comparison of simple linear data reconciliation methods

| Stream | Standard deviation | Measured value | Calculation value | | |
|--------------------------|--------------------|----------------|-------------------|---------|---------|
| | | | DATACON | GA | GSA |
| 1 | 1.001 | 100.1 | 99.287 | 99.400 | 99.288 |
| 2 | 0.822 | 41.1 | 41.1 | 41.1 | 41.1 |
| 3 | 0.790 | 79.0 | 79.359 | 79.321 | 79.361 |
| 4 | 1.530 | 30.6 | 30.048 | 29.938 | 30.042 |
| 5 | 2.166 | 108.3 | 109.407 | 109.271 | 109.403 |
| 6 | 0.396 | 19.8 | 19.927 | 20.083 | 19.927 |
| 7 | - | - | 58.187 | 58.3 | 58.188 |
| 8 | - | - | 38.259 | 38.217 | 38.261 |
| Objective function value | | | 1.362 | 1.5548 | 1.3619 |
| $F_1 - F_2 - F_7 =$ | | | 0 | 0 | 0 |
| $F_7 - F_6 - F_8 =$ | | | 0.001 | 0 | 0 |
| $F_2 + F_8 - F_3 =$ | | | 0 | 0.004 | 0 |
| $F_3 + F_4 - F_5 =$ | | | 0 | -0.012 | 0 |

Table 3. Redescending estimator tuning constant values for simple linear data reconciliation with error

| | M ₁ | M ₂ | M ₃ | M ₄ | M ₅ | M ₆ | M ₇ | M ₈ | Best solution |
|------------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|---------------|
| C | 40 | 20 | 16 | 8 | 4 | 2 | 0.8 | 0.4 | 1.65 |
| n _{out} | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 2 | 1 |
| OP | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 1 | 1 |
| AVTI | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 1 | 0 |
| AIC | 4.648E+05 | 4.648E+05 | 4.648E+05 | 4.648E+05 | 4.648E+05 | 4.648E+05 | 38.899 | 55.285 | 38.087 |
| F ₁ | 107.942 | 107.942 | 107.942 | 107.942 | 107.942 | 107.942 | 98.849 | 97.508 | 99.139 |
| F ₂ | 41.100 | 41.100 | 41.100 | 41.100 | 41.100 | 41.100 | 41.100 | 41.100 | 41.100 |
| F ₃ | 80.548 | 80.548 | 80.548 | 80.548 | 80.548 | 80.548 | 78.970 | 77.700 | 79.179 |
| F ₄ | 29.184 | 29.177 | 29.180 | 29.183 | 28.770 | 31.997 | 29.376 | 30.600 | 30.876 |
| F ₅ | 109.732 | 109.725 | 109.730 | 109.731 | 109.318 | 112.545 | 108.346 | 108.30 | 110.054 |
| F ₆ | 20.576 | 20.576 | 20.576 | 20.576 | 20.576 | 20.576 | 19.879 | 19.808 | 19.960 |
| F ₇ | 66.842 | 66.842 | 66.842 | 66.842 | 66.842 | 66.842 | 57.749 | 56.408 | 58.039 |
| F ₈ | 46.266 | 46.266 | 46.266 | 46.266 | 46.266 | 46.266 | 37.870 | 36.600 | 38.079 |

Let us assume another set of data from this same system with an error induced in the measurement of stream 1, with a value of 110.1 recorded instead of the previous value of 100.1. In general, the engineer would not know that such an error existed in the raw data. In this case, a redescending estimator is used as the objective function in the comparison of GSA, simple GA and DATACON, as summarized in Table 3.

Table 3 shows that the M₁ to M₆ cannot detect the outliers (n_{out} = 0). At M₇ the outlier starts to be detected, which can be seen from a sharp decrease in the AIC value. M₇ and M₈ detect 100% of the measurements as being corrupted. This is due to the increase in type 1 errors with increasing robustness of the estimator. The AIC also increases from M₆ to M₈. A plot of the AIC with the values of C shows a minimum at M₇, indicating that the best estimator lies close to it. With this

knowledge the estimator is tuned to C = 0.81. A comparison with the other methods is shown in Table 4.

There is no significantly different result in steam 1 with the introduced gross error. Here, the proposed technique gives the objective function value (2.437), which is not close to the DATACON result (0.221) because of the influence of the redescending estimator objective function. However, simultaneous gross error detection and reconciliation of data are performed well with the redescending estimator. In addition, DATACON normally performs data reconciliation using a global test and a measurement test to detect gross errors before continuing with data reconciliation.

5.4 Binary distillation column

This problem is a simple example of reconciled flows and compositions of a binary distillation column with no gross error in measured data (Narasimhan & Jordache, [1]).

The flows and component mole fractions of feed (F), distillate (D), and bottom streams (B) are measured. The measured flow rates under noise are based on data from 100 measurements, with 5% standard deviation.

The measured mole fractions are found in the same way, with 1% standard deviation from true values. A set of the true values, measured values, and standard deviations is presented in Table 5.

If we represent the value of the flow of feed, distillate and bottom streams by the variables EMBED Equation.3 and the measured compositions by the variables EMBED Equation.3, we will get one overall flow balance and two component balances, as follows:

$$x_F - x_B - x_D = 0$$

$$(8a) x_F y_{F1} - x_B y_{B1} - x_D y_{D1} = 0$$

$$(8b) x_F y_{F2} - x_B y_{B2} - x_D y_{D2} = 0$$

$$(8c) y_{F1} + y_{F2} = 1$$

$$(8d) y_{B1} + y_{B2} = 1$$

$$(8e) y_{D1} + y_{D2} = 1$$

$$(8f)$$

In this case, Wongrat [9] used a nonlinear constraint parameter with weighted least squares as the objective function in the comparison of GSA and GA. The result is shown in Table 5.

It can be seen that the GSA produces a better solution than the GA in Wongrat's study, in which the selection process was modified with CPSS. In principle, both techniques aim to improve the stage of selection of general GA, but the approach of simulated annealing in GA (GSA) seems to work more efficiently.

Table 4. Comparison of simple linear data reconciliation with error

| I | Standard deviation | Measured value | Calculation value | | |
|--------------------------|--------------------|----------------|-------------------|---------|---------|
| | | | DATACON | GA | GSA |
| 1 | 1.101 | 110.1 | 98.694* | 98.609* | 99.139* |
| 2 | 0.822 | 41.1 | 41.1 | 41.1 | 41.1 |
| 3 | 0.790 | 79.0 | 78.894 | 79.046 | 79.179 |
| 4 | 1.530 | 30.6 | 30.203 | 30.004 | 30.876 |
| 5 | 2.166 | 108.3 | 109.097 | 109.063 | 110.055 |
| 6 | 0.396 | 19.8 | 19.800 | 19.571 | 19.960 |
| 7 | - | - | 57.594 | 57.509 | 58.039 |
| 8 | - | - | 37.794 | 37.938 | 38.079 |
| Objective function value | | | 0.221 | 4.786 | 2.437 |
| $F_1 - F_2 - F_7 =$ | | | 0.000 | 0.000 | 0.000 |
| $F_7 - F_6 - F_8 =$ | | | 0.000 | 0.000 | 0.000 |
| $F_2 + F_8 - F_3 =$ | | | 0.000 | -0.008 | 0.000 |
| $F_3 + F_4 - F_5 =$ | | | 0.000 | -0.013 | 0.000 |

Table 5. Comparison of GA and GSA results for a binary distillation column

| Stream | Variables | STD | Measured value | Calculation value | |
|--|-----------------|----------|----------------|-------------------|----------|
| | | | | GA by Wongrat | GSA |
| | | | | WLS | WLS |
| Feed | Flow | 50.000 | 1006.3 | 1003.62 | 1003.530 |
| | Component 1 (%) | 0.480 | 48.060 | 48.047 | 47.991 |
| | Component 2 (%) | 0.520 | 52.065 | 52.028 | 52.009 |
| Distillate | Flow | 24.731 | 497.72 | 496.261 | 496.262 |
| | Component 1 (%) | 0.950 | 95.119 | 95.145 | 95.003 |
| | Component 2 (%) | 0.050 | 4.998 | 4.998 | 4.997 |
| Bottom | Flow | 25.269 | 504.470 | 507.359 | 507.268 |
| | Component 1 (%) | 0.020 | 1.999 | 1.980 | 1.999 |
| | Component 2 (%) | 0.980 | 97.965 | 98.029 | 98.001 |
| Objective function value | | - | 0.93273 | 0.06773 | |
| $x_F - x_B - x_D = 0$ | | 4.038 | 0.000 | 0.000 | |
| $x_F y_{F1} - x_B y_{B1} - x_D y_{D1} = 0$ | | 0.117 | -0.004 | 0.001 | |
| $x_F y_{F2} - x_B y_{B2} - x_D y_{D2} = 0$ | | 4.850 | 0.001 | -0.001 | |
| $y_{F1} + y_{F2} = 1$ | | 100.125% | 100.075% | 100% | |
| $y_{B1} + y_{B2} = 1$ | | 100.117% | 100.143% | 100% | |
| $y_{D1} + y_{D2} = 1$ | | 99.964% | 100.009% | 100% | |

Table 6. Refinery problem results – mass and energy balance

| i | Variable | Standard deviation | Measured value | Calculation value | |
|--------------------------|----------------|--------------------|----------------|-------------------|---------|
| | | | | DATACON | GSA |
| 1 | Rate, ton(s)/h | 6.600 | 330.000 | 322.970 | 322.951 |
| | Temp, °C | 1.00 | 154.00 | 154.662 | 154.723 |
| 2 | Rate, ton(s)/h | - | - | 131.696 | 131.537 |
| | Temp, °C | - | - | 154.662 | 154.723 |
| 3 | Rate, ton(s)/h | - | - | 191.274 | 191.414 |
| | Temp, °C | - | - | 154.662 | 154.723 |
| 4 | Rate, ton(s)/h | 2.640 | 132.000 | 131.696 | 131.537 |
| | Temp, °C | 1.00 | 170.00 | 170.492 | 170.531 |
| 5 | Rate, ton(s)/h | 3.840 | 192.000 | 191.274 | 191.414 |
| | Temp, °C | 1.00 | 185.00 | 185.339 | 185.376 |
| 6 | Rate, ton(s)/h | - | - | 322.970 | 322.951 |
| | Temp, °C | - | - | 179.339 | 179.388 |
| 7 | Rate, ton(s)/h | - | - | 322.970 | 322.951 |
| | Temp, °C | 1.00 | 221.00 | 219.346 | 219.464 |
| 7A | Rate, ton(s)/h | - | - | 322.970 | 322.951 |
| | Temp, °C | - | - | 322.970 | 322.951 |
| 8 | Rate, ton(s)/h | 1.360 | 68.000 | 67.914 | 67.855 |
| | Temp, °C | 1.00 | 200.00 | 200.061 | 200.040 |
| 9 | Rate, ton(s)/h | 1.320 | 66.000 | 65.969 | 65.899 |
| | Temp, °C | 1.00 | 285.00 | 285.213 | 285.205 |
| 10 | Rate, ton(s)/h | 1.300 | 65.000 | 65.365 | 65.352 |
| | Temp, °C | 1.00 | 121.000 | 123.722 | 123.845 |
| 11 | Rate, ton(s)/h | 2.420 | 370.00 | 370.693 | 370.700 |
| | Temp, °C | 1.00 | - | 123.722 | 123.845 |
| 12 | Rate, ton(s)/h | - | - | 274.378 | 274.325 |
| | Temp, °C | 1.00 | 275.00 | 65.365 | 65.352 |
| 13 | Rate, ton(s)/h | - | - | 199.810 | 199.800 |
| | Temp, °C | 1.00 | 200.00 | 65.969 | 65.899 |
| 14 | Rate, ton(s)/h | - | - | 168.941 | 168.969 |
| | Temp, °C | 1.00 | 169 | 7.01896 | 7.0022 |
| Objective function value | | | | | |

5.5 Simple refinery

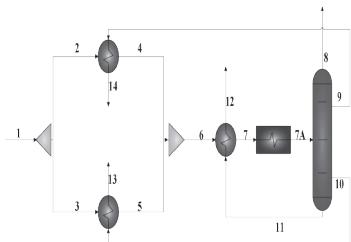


Fig. 4. Simple refinery.

The measured values for the case in Fig. 4 are shown in Table 6 with a 2% standard deviation of measurement. The product streams consist of one component per stream, except for the overhead Naphtha product which contains five pure components and one heavy pseudo-component. This complex case study has bilinear constraints. The weighted least squares method is used as the objective function in the comparison of GSA and DATACON. It can be seen that the simultaneous mass and energy constraint produces better results for complex DR from GSA (7.0022) than from DATACON(7.01896).

6 Conclusion

An optimization tool using GSA for DR problems has been presented. The GSA based program is the optimization tool for data reconciliation using two kinds of objective function. The weighted least square objective function is used for data reconciliation and the redescending estimators and the modified AIC objective function are used for data reconciliation of measured data contained gross error by developing code program

in MATLABTM for the difficulty of complex problems. GSA has a better searching ability for the global optimal solution. GSA generates a new individual with GA; then these individuals are processed with SA, and the results are used as the initial individuals of the next generation. The systematic approach of GSA to the DR problem was proposed and implemented. This method started with appropriate GSA parameter formulation and then used these parameters to solve the DR problem. The steady-state DR problem was tested with this proposed program. The results showed that the GSA method could be a promising choice as an optimization tool for the DR problem, with the ability to give more accurate reconciled data.

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NOMENCLATURE

AIC : Akaike information criterion

AVTI : Average number of type 1 errors

a, b, c : Tuning constants for the redescending estimator

DR : Data reconciliation

ΔE : Difference of fitness values between the child generation and the parent generation

F : Feed flow rate

GA : Genetic algorithm

GSA : Genetic simulated annealing algorithm

g : The set of inequalities constraints

h : The set of equality constraints

N : Number of variables

n : Total number of measured variables

nout : Total number of detected gross error

P : Probability

OP : Optimization of Probability

SA : Simulated annealing

u : The set of unmeasured variables

WLS : Weighted least squares

x^M : The set of measured variables

x : The set of reconciled values

M : Measured value

ϵ : The magnitude of random error

ρ : Some objective function dependent upon the difference between the measurement of a variable and its value for any measured variables

Superscripts

L : Lower bound of variable

U : Upper bound of variable

Subscripts

i : Variable index