A MIXED INTEGER NONLINEAR OPTIMIZATION BASED APPROACH TO SIMULTANEOUS DATA RECONCILIATION AND BIAS IDENTIFICATION

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Abstract

The problem of data reconciliation and the detection and identification of gross errors, such as measurement bias, are closely related and permits a solution within a mixed integer optimization framework. A mixed-integer linear programming (MILP) approach has been previously investigated by Soderstrom et al. (2001), where the process model was described by a set of linear equations. This paper outlines an extension of that technique when the model contains only bilinear terms as well as general nonlinear ones, requiring the solution of a mixed integer nonlinear program (MINLP). Several solution methods were compared including the outer approximation / equality relaxation algorithm implemented in GAMS, genetic algorithms, and Tabu Search. These methods were tested on several challenging test problems, showing an improvement over other published methods for bias detection.

Keywords

Gross Error Detection, Data Reconciliation, Bias Identification, Mixed-integer Nonlinear Programming

Introduction

Plant data are often corrupted by random and gross errors, so it is beneficial to use data reconciliation techniques combined with physical models of the unit operations to estimate values of measurements consistent with material and energy balances. Because plant models can be nonlinear and gross errors can be viewed as a 0-1 occurrence, methods based on mixed integer nonlinear programming would be useful to solve the complete problem. We use a formulation where gross error detection and data reconciliation can be carried out simultaneously.

Eqn. (1) gives a formal statement of the MINLP considered here. This problem penalizes solutions with large absolute deviations from measured values and a large number of identified biases. The formulation in Eqn. (1) does not explicitly contain the absolute value error, which prevents a single outlier from skewing the results or forcing a bias to be falsely identified.

$$
\begin{aligned}
&\min_{\substack{\mu_i, B_i, S_i \\ \delta_i, p_{ik}, n_{ik}}} \Phi = \sum_{k=1}^{h}\sum_{l=1}^{n}\frac{1}{\sigma_l}\left(p_{lk}-n_{lk}\right)+\sum_{l=1}^{n} w_l B_l \\
&\text{s.t} \quad \mathbf{f}\left(\boldsymbol{\mu},\mathbf{x}\right)=\mathbf{0} \\
&\qquad \mu_l-\left(y_{lk}-\delta_l\right)=p_{lk}-n_{lk} \\
&\qquad \delta_l-U_l B_l\le 0 \\
&\qquad -\delta_l-U_l B_l\le 0 \\
&\qquad \delta_l-S_l\left(1+\varepsilon_l\right)U_l+\varepsilon_l U_l B_l\le 0 \\
&\qquad -\delta_l+S_l\left(1+\varepsilon_l\right)U_l+\varepsilon_l U_l B_l\le\left(1+\varepsilon_l\right)U_l \\
&\qquad S_l-B_l\le 0 \\
&\qquad p_{lk}, n_{lk}, \mu_l\ge 0 \quad B_l, S_l\in binary
\end{aligned}
\tag{1}
$$

The p and n variables represent positive and negative deviations, while the σ and w variables can be thought of as weighting factors. The sign and existence of a bias are expressed through the binary variables S and B

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respectively. The measured and unmeasured variables are represented by μ and x respectively.

In Eqn. (1) B_l represents the existence of a bias in the lth measurement, and w_1 is a weighting factor for the lth binary variable. The weighting factor is a positive number chosen to change the importance of finding solutions with the smallest possible number of biased measurements identified. As long as the weighting factor is chosen so that a bias of the minimum size considered would inflate the value of the objective function more than the weighting factor for the biased measurement, the solution is relatively insensitive to the choice. Here the variable U_l is a large number which can be viewed as an upper limit on the magnitude of bias considered. The second set of constraints ensures that the magnitude of any bias will be zero if the associated binary variable is not activated. The third set requires any bias to be of a certain magnitude before it is considered important. The value of ε_l can be some scaling factor related to the precision of the measurement. If the term, ε_l, is chosen such that the quantity of $\varepsilon_l\ U_l$ is some fraction of the standard deviation of the measurement, this would eliminate cases where a bias would be small relative to the measurement error.

Conceptually the extension of the MILP method for simultaneous data reconciliation and bias detection/identification of linear models to nonlinear models is straightforward. However, once nonlinear equations are introduced, the optimization problem, a mixed integer nonlinear program (MINLP), is a tougher class of problem whose solution technology is not as advanced or mature as for MILP.

A general MINLP can have nonlinear terms in the objective and constraints, in both the continuous and discrete variables. However, if the problem to be solved has specific features, often special algorithms exist that may be more successful at solving a particular problem. In this paper we compare three methods chosen to solve the MINLP.

Outer Approximation / Equality Relaxation

The Outer Approximation / Equality Relaxation (OA/ER) algorithm was proposed by Kocis and Grossman (1987) and is described in detail by Floudas (1995). This algorithm is designed to solve MINLP problems where the integer variables only appear linearly in the objective and constraints. The mixed integer bias detection problem is of this type and can be solved using an algorithm such as DICOPT^{++}, which has an interface to GAMS.

Genetic Algorithms

The genetic algorithm (GA) is a common derivative-free optimization technique which has been applied to a wide variety of both continuous and discrete problems. For this problem GA was used to search over combinations of the binary variables. Once their values were fixed, the underlying NLP was solved. Genetic algorithms are a population-based method so a number of solutions are retained and new solutions are generated from the existing population using a series of operations. The operations include selection, mutation and crossover (Reeves, 1997).

Perhaps the most important part of using a genetic algorithm is choosing an encoding scheme. In the data reconciliation / bias identification problem, there are two sets of binary variables. The problem is set up such that the first set signifies whether or not a bias is present, and the second set determines the sign of the bias. In order to avoid a solution uniqueness problem with the second set of binary variables, binary variables are encoded, and the constraints are selected to force a variable from the second set to have a value of zero if the corresponding member of the first set has a value of zero, thus achieving feasibility.

A population member is produced by concatenating n bytes of length 2 and treating each byte as an element in the vector. The byte in position i can be thought of as an ordered pair consisting of the associated binary variables for measurement i, chosen from the set κ.

$$\kappa \equiv \{(0,0),(1,0),(1,1)\} \tag{2}$$

These bytes are chosen randomly to form an initial population. Crossover and mutation can be easily specified such that the parent can only break at a location where two bytes join, thus all offspring will be feasible as well. When mutations occur at a location, the mutation is chosen from the set κ as well. This will ensure that any mutation will produce potentially feasible combinations of binary variables as well.

Tabu Search

The Tabu Search (TS) method described by Glover and Laguna (1997) has a metaheuristic procedure, which directs a search method (e.g., a descent method) into regions that would remain unexplored with a traditional search algorithm. TS can solve hard combinatorial problems because it allows for sequences of non-improving moves and can easily break out of local minima while seeking the global optimum. In this problem, the search portion was performed on the binary variables in (1) and the NLP solver was used to find an optimal solution for the continuous variables.

Defining a neighborhood of the solution is very important because a TS evaluates several solutions in some neighborhood of the current solution, choosing the best one (but not necessarily the one with the lowest objective value). Here a solution is a n×1 vector with each entry a "state" corresponding to a measurement. Each state has three possible combinations of binary variables (B_i,Y_i) as shown in Eq. 2. The neighborhood of a solution is defined as any solution generated from the current solution by changing the state of any single element.

We now apply the three techniques discussed above on two examples from the literature.

Nonlinear CSTR Example

The system chosen to test the MINLP approach is an adiabatic CSTR used by Kim et al. (1997) to test another gross error detection method. The reaction carried out is a first order reversible reaction with single species reactants and products. It was assumed that all variables were measured and the measurements were independent with a standard deviation of 0.025 for the concentrations and 3.0 for the temperature. As was done in Soderstrom et al. (2001), Monte Carlo simulation was used to test the performance of the method on nonlinear systems. The sign, location of the bias, and the magnitude were all varied randomly for each trial. The magnitude of the bias was allowed to vary from 10% to 100% of the true value of the variable. For each set of trials, the number of biased measurements was fixed at either one, two, or three.

The same performance measures, overall power (OP) and average Type I errors (AVTI), were used to evaluate the performance of the MINLP method. OP is a measure of the fraction of biases correctly identified and AVTI is related to the number of unbiased variables incorrectly identified as biased. The results of a series of simulations are shown in Table 1.

These results show a very high power for identifying the biased variable or variables correctly with very few false identifications as shown by the low value of the AVTI. This example shows only the results of solving the problem using the OA/ER method. A comparison of the other methods will be shown in the next example, which has a larger number of variables. In several cases, when a misidentification occurred in a run, it was noted that the solver failed to find the combination which produced the lowest objective value. This was verified by fixing the binary variables in the combination representing the true set of biased variables and solving the NLP. This occurrence increased as the number of binary variables increased.

Table 1: Solution for MINLP technique Using OA/ER GAMS Implementation

Horizon Length	# Biased	OP	AVTI
10	1	0.960	0.01
	2	0.915	0.03
	3	0.923	0.07

Because it is possible to bound the estimates, the MINLP method was compared to another bias detection method employing bounded estimates. These bounds did not force the solver to find a solution with a higher objective function than when less constrained, but usually the bounds prevented the solver from diverging and kept the solver on track on this highly nonlinear problem. This same problem was used in a simulation study of the modified iterative measurement (MIMT) test using NLP techniques by Kim et al. (1997).

In their formulation, the data reconciliation step of the method was solved with a NLP solver with bounds imposed on the estimates. In their study, estimates of the measurements were bounded at ±20% of the true value. Even with these stricter bounds the MINLP method performs significantly better with a larger OP and smaller AVTI, as shown in Table 2.

Table 2: Comparison of MINLP and MIMT

	MIMT		MINLP	
# Biased Measurements	1	2	1	2
OP	0.87	0.87	0.96	0.92
AVTI	0.08	0.31	0.01	0.03

Both methods do a good job of identifying the correct biased measurement, however, the clear advantage of the MINLP method is the low number of Type I errors.

Heat Exchanger Network Example

The second example to test the performance of the various MINLP solution techniques, a heat exchanger network used by Albers (1994) for gross error detection tests, was examined. A diagram of the system is shown in Fig. 1.

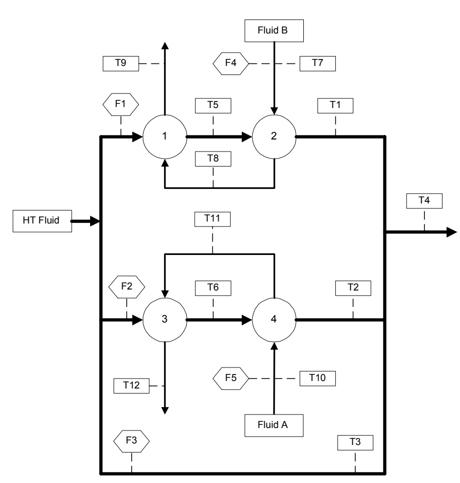

Figure 1: Heat Exchanger Network

The model of the system consists of steady state material and energy balances with the enthalpies of the various streams expressed as functions of the temperature, making the model nonlinear. The values of the constants and measured variables as well as the standard deviation of the measurements are the same as in the article.

As in the previous example, a series of Monte Carlo simulations were performed on this system using the OA/ER, TS, and genetic algorithm methods to solve the MINLP problem. The sign, location of the bias, and the magnitude were all varied randomly for each trial. The magnitude of the bias was allowed to vary from 10% to 100% of the true value of the variable. For each set of trials, the number of biased measurements was fixed at either one, three, or five.

All methods involve solving NLP subproblems with a fixed combination of binary variables, so the same solver settings and bounds were used for all methods. A horizon length of 10 was chosen and variable estimates were bounded to be ±50% of the true value. The performance of the various methods is shown in Tables 3 and 4.

Table 3: Comparison of Solution Methods

# of Biased Variables	Overall Power		
	OA/ER	Tabu Search	GA
1	0.97	0.97	0.91
2	0.92	0.93	0.82
3	0.94	0.91	0.73

Table 4: Comparison of Solution Methods

# of Biased Variables	Average Type I Errors (AVTI)		
	OA/ER	Tabu Search	GA
1	0.05	0.10	0.51
2	0.16	0.26	0.59
3	0.18	0.38	0.53

Although both the OA/ER method and the TS clearly have the highest OP and lowest AVTI, there are other considerations, for example the TS requires many more NLP subproblems to be solved. Typical results for the number of NLP's solved are shown in Table 5.

Table 5: Comparison of the Typical Number of NLP Subproblems Required

Solution Method	# NLP Subproblems
OA/ER	4
Tabu Search	362
GA	1000

The number of NLP subproblems was always the same because in this implementation the number of generations and population size was fixed. The OA/ER method almost always converged within three major iterations after solving the relaxed problem. The method showing the most variation was the TS. The stopping criterion for the TS was the number of restarts without improvement. After this limit was reached, the search was terminated. This number must be chosen carefully; if it is too small, the search may end without finding the optimal solution. The TS is a purposeful search and as long as the objective is improving between restarts, the search will continue. The best performance of the method was obtained when the current best solution was used as the initial point upon restart.

In a few cases, TS found a solution where OA/ER did not find the correct biases. Normally, the optimal solution for TS was found within the first few moves. The initial combination of binary variables is obtained by rounding the binary variables in solution of the relaxed problem to the nearest integer. Sometimes this does not always start the solution off in a neighborhood of the minimum and more iterations and restarts are required. Non-improving moves are often accepted, allowing the search to break out of local minima.

For all three methods, the computational tests showed that the minimum gross error size is fairly unimportant in practice and may be left out of the formulation. The choice of the weighting factors for the binary variables has more of an influence. If the active binary variable weighting factor is chosen so that its contribution to the objective is greater than the weighted measurement residuals contribution to the objective (until the residual is of a minimum size), there is less of a penalty for choosing the solution with lower gross errors identified. This prevents a small magnitude gross error from being identified. Setting the minimum size threshold really seems to improve the chances of finding the best solution. Not changing the combination of gross errors identified leads to the smallest objective. The search over the binary variables seems to proceed more efficiently when this is incorporated into the problem.

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