AIChE Wiley InterScience

A New and Improved MILP Formulation to Optimize Observability, Redundancy and Precision for Sensor Network Problems

Jeffrey D. Kelly and Danielle Zyngier
Honeywell Process Solutions, 300 Yorkland Blvd., North York, ON, Canada

DOI 10.1002/aic.11475
Published online March 26, 2008 in Wiley InterScience (www.interscience.wiley.com).

New mathematical formulations of observability, redundancy, and an improved formulation for precision are provided which can be explicitly and analytically solved using mixed integer linear programming (MILP). By using the Schur complement found at the heart of both Gaussian elimination and Cholesky factorization for direct block matrix reduction and the variable classification and covariance calculations found in the reconciliation, regression, and regularization approach of Kelly, it is possible to efficiently optimize the overall instrumentation cost considering both estimability and variability as constraints during the branch-and-bound search of the MILP. Two illustrative examples are highlighted which minimize the cost of sensor placement subject to software and hardware redundancy of the measured variables, observability of the unmeasured variables, and their precision (i.e., inverse of their variance). This formulation is well suited to the problems of designing as well as retrofitting sensor locations in arbitrary networks. © 2008 American Institute of Chemical Engineers *AIChE J,* 54: 1282–1291, 2008
Keywords: reconciliation, regression, error-in-variables, implicit models, estimability, variability, Schur complement, sensor network location

Introduction

Determining what sensors, instruments, analyzers, meters, or field devices to install during the design or retrofit stages of the construction process can be a tedious and uncertain task. This article proposes a new mixed integer linear programming (MILP) formulation which has the ability to simultaneously consider three important aspects of any sensor network or superstructure found in the process industries. The term "superstructure" is somewhat preferred over "network" given that a superstructure is an arbitrary combination of one or more networks as in the case of process synthesis and scheduling problems where different options and operations can exist dependent on diverse design and dispatch decisions. However, for the purposes of this work, networks are studied although the analysis can be applied equally to superstructures.

Correspondence concerning this article should be addressed to J. D. Kelly at Jeff.Kelly@honeywell.com.

The first two important aspects of a sensor network are variable observability and redundancy which have been well studied in the literature on data reconciliation.[1–9] Bagajewicz[9] defines the general term "estimability" referring to the assessment of any variable that is estimable if it is measured or unmeasured but observable. The third important aspect of a sensor network is that of estimating precision or variability. For instance, an unmeasured variable may be observable, but given the available measured variables and material, energy, and momentum balances, it is regressed from its variability may be unacceptably high. The only way to improve or increase its precision is to (a) record it directly with a sensor (if possible), (b) add other sensors it is spatially related to, (c) replace some sensors with more precise sensors, and/or (d) include more law of conservation equations.* In essence, the major focus of optimal sensor location problems is to determine from the list of (a), (b), or (c) [usually given a fixed set of balance equations (d)] what variables should be measured and what variables should be unmeasured given the pecuniary or monetary resources available subject to estimability and variability constraints. These types of problems are an active area of research which also may include other aspects of the problem such as recognition, reliability, resilience, robustness, resolution, repairability, residual precision, etc.[9–20]

The focus of this work is to highlight a new MILP approach that is general enough to address simultaneously and explicitly the observability, redundancy (estimability), and precision (variability). In the previous literature on the design and upgrade of sensor networks or superstructures, a mathematical programming approach to ensure observability and redundancy had not been derived. Hence, ad hoc evolutionary and enumeration-tree searches are used such as those found in the works of Bagajewicz[12] and Carnero et al.[13,14] as well as in that of Gala and Bagajewicz[20] who employ cutsets. As will be shown, these ad hoc approaches are not necessary in solving the estimability problem when the variable classification method of Kelly[1] and the Schur complement[21–23] are used. In addition, when optimizing cost subject to precision or variability constraints is the goal such as in the works of Bagajewicz and Cabrera[16] and Chmielewski et al.,[17] sophisticated MILP and linear matrix inequality formulations are used to parameterize the diagonal of the covariance matrices as functions of the sensor location logic variables (measured vs. unmeasured). Unfortunately, these approaches involve a very large number of variables and constraints and are only appropriate for small to medium-sized problems. The approach in this work is to also use MILP but to exploit the sparsity of the regularization kernel matrix of Kelly,[1] which also has at its foundation the useful concept that unmeasured variables can be included as measurements with infinite variance which is the key assumption used in the two other approaches mentioned.

Observability, Redundancy, and Precision MILP Formulations

Initially a model is needed that represents the network and this is contained in the variables' incidence matrix denoted as D of row size NG and column size NXY. For linear problems such as the ones that consider steady-state material balances, D is sparse and is usually composed of 1s and -1s. If the problem is nonlinear then the D matrix is still sparse and its elements are replaced by the Jacobian matrix elements. In the data reconciliation literature, it is well known that D is usually partitioned into two smaller A and B matrices with the same number of rows of size NG but a smaller number of columns of size NX and NY (number of measured and unmeasured variables respectively).[1] The fixed† variables' C incidence matrix of column size NZ is neglected because it does not contribute to the estimability or the variability of the problem. For the estimability constraints we need to define for convenience the $D^{T}D$ matrix which is represented and computed as

$$\mathrm{DTD}_{j,jj} = \sum_{i=1}^{\mathrm{NG}} D_{i,j} \cdot D_{i,jj}, \quad j,jj = 1 \ldots \mathrm{NXY} \tag{1}$$

where DTD corresponds to the $D^{T}D$ matrix, i in this case is the index of the rows or equations and j and jj are the indices of the columns or variables. It is also possible to scale DTD before generating the MILP constraints following the technique found in the work of Kelly[1,24] or by scaling DTD by the square-root of its diagonal elements.

We first present the objective function of the problem which is purely cost-based. The objective is to minimize the overall instrumentation cost as well as costs associated with not satisfying the constraints, i.e., the cost for a sensor $p_{\alpha,j}$, the cost for one additional sensor for the same variable $p_{\beta,j}$ required for hardware redundancy‡ considerations, and the provisional elastic, artificial, or penalty costs ru_j, rv_j, and rw_j for observability, redundancy, and precision violations if they occur.

$$\underset{\alpha_j,\beta_j}{\text{Minimize}} \sum_{j=1}^{\mathrm{NXY}} (p_{\alpha,j} \cdot \alpha_j + p_{\beta,j} \cdot \beta_j + ru_j \cdot eu_j + rv_j \cdot ev_j + rw_j \cdot ew_j) \tag{2}$$

The primary binary variable α_j is 1 if the variable is measured and a 0 if the variable is unmeasured whereby an unmeasured variable has no cost contribution. The secondary binary variable β_j denotes a practical requirement for a secondary sensor in order to maintain hardware redundancy especially when the reliability of the primary but usually lower-cost sensor is poor. The variable β_j can only be 1 if α_j is 1 (restricted by a simple sequence-dependency constraint in the redundancy constraint set). The error variables eu_j, ev_j, and ew_j are nonnegative, and if all estimability and variability constraints are satisfied, they will be zero at an integer-feasible MILP solution. There are no singleton upper bounds applied to the nonnegative error variables given that they are minimized in the objective function with nonnegative weights and hence unboundedness will not occur.

The set of observability constraints below is new to the literature on sensor design and retrofit problems. The mathematical formulation of these constraints is taken from the approach used by Kelly[23] to find the matrix projection of Crowe et al.[25] called the "recursive matrix inversion by partition." This technique involves systematically, one column of B at a time, checking for a near-zero Schur complement[21,22] of the partitioned $B^{T}B$ matrix which is computed in an identical manner to DTD in Eq. 1. Given that it is well known that if the Schur complement is zero then the determi-

* Unfortunately these may introduce more uncertainty with respect to their structure and parameterization.

† Fixed variables are not really variables but parameters given that they are known exactly.

‡ There is software redundancy which requires the model, and hardware redundancy which requires a secondary sensor.

nant of the matrix in question is zero then in this case the matrix is declared to be singular or noninvertible (Cramer's rule). This implies that the column of B is somehow linearly dependent on other columns of B in the set of all unmeasured variables hence making it unobservable by definition.[1,5] In the variable classification section of Kelly,[1] it is shown that if any linearly dependent columns of B exist, then all of these columns relating to the unmeasured variables are unobservable (see Appendix). Thus, our approach in this article is to systematically check en bloc in the MILP each unmeasured variable (if $\alpha_j = 0$) for any linearly dependency in the DTD matrix relating to other unmeasured variables only. This is articulated mathematically in constraint set 3.

$$\mathrm{DTD}_{i,j} \cdot (1-\alpha_j) - M \cdot \alpha_i \le \sum_{\substack{ii=1 \\ ii \ne j}}^{\mathrm{NXY}} \mathrm{DTD}_{i,ii} \cdot u_{ii,j} \le \mathrm{DTD}_{i,j} \cdot (1-\alpha_j) + M \cdot \alpha_i, \quad i,j = 1 \ldots \mathrm{NXY},\ i \ne j \tag{3a}$$

$$-M \cdot (1-\alpha_i), \le u_{i,j} \le M \cdot (1-\alpha_i), \quad i,j = 1 \ldots \mathrm{NXY},\ i \ne j \tag{3b}$$

$$-M \cdot (1-\alpha_j), \le u_{i,j} \le M \cdot (1-\alpha_j), \quad i,j = 1 \ldots \mathrm{NXY},\ i \ne j \tag{3c}$$

$$(1-\alpha_j) - (1/\mathrm{DTD}_{j,j}) \cdot \sum_{\substack{i=1 \\ i \ne j}}^{\mathrm{NXY}} \mathrm{DTD}_{j,i} \cdot u_{i,j} \ge (1-\alpha_j) \cdot (1/\mathrm{DTD}_{j,j}) \cdot \varepsilon_u - eu_j, \quad j = 1 \ldots \mathrm{NXY} \tag{3d}$$

$$eu_J \le M \cdot (1-\alpha_j), \quad j = 1 \ldots \mathrm{NXY} \tag{3e}$$

The observability working variable u is a two-dimensional free variable of row and column size NXY, ε_u is an observability tolerance which may be defined for each variable (usually set to 10^{-3}) and M (also referred to as "big M") can be either arbitrarily specified or a tighter estimate can be determined as the largest absolute nonzero value of any individual element or element inverse found in DTD. Constraints 3b and 3c will force the working variable $u_{i,j}$ to be zero if it corresponds to any measured variable meaning that it is not part of the set of unmeasured variables. Constraint 3d is scaled by the diagonal elements of DTD where if the unmeasured variable is not observable then constraint 3d is provisionally relaxed using the error variable eu. Constraint 3e is added for improving the efficiency of the method in that it states that there are no observability errors if the variable is measured. Constraint set 3 can also be used for standard data reconciliation solving to classify unmeasured variables as observable or unobservable when the partitions of D into A and B are already known exogenously.

Interestingly and as a matter of insight, if the α_js are known, it is also possible to determine observable unmeasured variables by checking the feasibility of the equations $B \cdot u = 0$ where $u_{i,i} = 1$ and the rest of the working variables are free. When a particular $u_{i,i}$ is set to 1 (indicating an unmeasured variable i), if a solution to the set of equations exists then this unmeasured variable is linearly dependent given that other unmeasured variables can be used to satisfy the equations $B \cdot u = 0$. This technique was used to confirm the solutions for the observability assessments in the illustrative examples.

The redundancy set of constraints are also new and is in spirit similar to the observability constraint set. It requires some modifications although both constraint sets use the Schur complement at their core. A detailed derivation of another approach to classify measured variables as a either redundant or nonredundant is presented in the work of Kelly,[1] where a true idempotent projection matrix denoted by E was introduced which was only a function of the partitions of B. By checking for nonzero diagonals of $A^{\mathrm{T}} \cdot E \cdot A$ it is possible to determine redundant measured variables (see Appendix). In addition, Kelly[2] later exploited this new projection matrix and developed a new and numerically robust data reconciliation algorithm using singular value decomposition (SVD) as well as expanding on the variable classifications using SVD and pseudoinverses. The redundancy constraint set is presented below.

$$\mathrm{DTD}_{i,j} - M \cdot \alpha_i - M \cdot (1-\alpha_j) \le \sum_{\substack{ii=1 \\ ii \ne j}}^{\mathrm{NXY}} \mathrm{DTD}_{i,ii} \cdot v_{ii,j} \le \mathrm{DTD}_{i,j} + M \cdot \alpha_i + M \cdot (1-\alpha_j), \quad i,j = 1 \ldots \mathrm{NXY},\ i \ne j \tag{4a}$$

$$-M \cdot (1-\alpha_i) \le v_{i,j} \le M \cdot (1-\alpha_i), \quad i,j = 1 \ldots \mathrm{NXY},\ i \ne j \tag{4b}$$

$$-M \cdot \alpha_j \le v_{i,j} \le M \cdot \alpha_j, \quad i,j = 1 \ldots \mathrm{NXY},\ i \ne j \tag{4c}$$

$$\alpha_j - (1/\mathrm{DTD}_{j,j}) \cdot \sum_{\substack{i=1 \\ i \ne j}}^{\mathrm{NXY}} \mathrm{DTD}_{j,i} \cdot v_{i,j} \ge \alpha_j \cdot (1/\mathrm{DTD}_{j,j}) \cdot \varepsilon_v - M \cdot \beta_j - ev_j, \quad j = 1 \ldots \mathrm{NXY} \tag{4d}$$

$$\alpha_j - (1/\mathrm{DTD}_{j,j}) \cdot \sum_{\substack{i=1 \\ i \ne j}}^{\mathrm{NXY}} \mathrm{DTD}_{j,i} \cdot v_{i,j} \le \alpha_j \cdot (1/\mathrm{DTD}_{j,j}) \cdot \varepsilon_v + M \cdot (1-\beta_j), \quad j = 1 \ldots \mathrm{NXY} \tag{4e}$$

$$\beta_j - \alpha_j \le 0, \quad j = 1 \ldots \mathrm{NXY} \tag{4f}$$

Constraint 4a is a disjunctive constraint in that if the j variable in question is an unmeasured variable then the constraint is trivialized or relaxed. Constraints 4b and 4c have similar explanations to the observability constraints which correspond to the big M constraints to fix the working variables v to 0 or to set them free if they are either measured or unmeasured, respectively. Constraints 4d and 4e correspond to the redundancy constraints where 4e includes the details around managing the hardware redundancy. Constraint 4f is the simple sequence-dependency constraint that only allows hardware redundancy when the variable has already been declared as measured. Finally, it should be emphasized that the observability and the redundancy problems do not require sensor precision estimates given that the estimability problem is purely a structural problem. However, this is not true for the variability problem below which does require estimates of the installed sensors precision to be known a priori.

Constraint set 5 presents the MILP formulation for the precision problem. Kelly[1] presents another derivation of the measured and unmeasured variable covariances which uses a sparse kernel matrix K equal to ($A \cdot Q \cdot A^T + \lambda \cdot B \cdot B^T$), where λ is an appropriately chosen large positive number which can be determined according to guidelines provided in the work of Kelly.[1] The variable λ can also be likened to a regularization parameter which practically represents the largest variance of any unmeasured variable and is identical in spirit to both the approaches of Bagajewicz and Cabrera[15] and Chmielewski et al.,[17] who assume that this variance is some very large number. The improvement in this MILP formulation over specifically that of Bagajewicz and Cabrera[15] is that we exploit the sparsity of K where we do not create free variables representing the inverse of K explicitly. The inverse of the kernel matrix used in the work of Bagajewicz and Cabrera[15] will be more dense than sparse because of fill-ins which can be easily observed when any direct or iterative factorization method such as Gaussian elimination or Cholesky factorization is used to calculate the inverse explicitly or any sparse matrix.

$$\sum_{jj=1}^{NXY}\sum_{ii=1}^{NG}[D_{i,jj} \cdot D_{ii,jj} \cdot (Q_{jj} \cdot w1_{ii,j} + (\lambda - Q_{jj}) \cdot w3_{ii,jj,j})] = Q_j \cdot D_{i,j} + (\lambda - Q_j) \cdot (1 - \alpha_j) \cdot D_{i,j}, \quad i = 1 \ldots NG,\ j = 1 \ldots NXY \tag{5a}$$

$$-M \cdot \alpha_{jj} + w1_{i,j} \le w3_{i,jj,j} \le M \cdot \alpha_{jj} + w1_{i,j}, \quad i = 1 \ldots NG,\ j, jj = 1 \ldots NXY \tag{5b}$$

$$-M \cdot (1 - \alpha_{jj}) \le w3_{i,jj,j} \le M \cdot (1 - \alpha_{jj}), \quad i = 1 \ldots NG,\ j, jj = 1 \ldots NXY \tag{5c}$$

$$-M \cdot \alpha_j + w1_{i,j} \le w2_{i,j} \le M \cdot \alpha_j + w1_{i,j}, \quad i = 1 \ldots NG,\ j = 1 \ldots NXY \tag{5d}$$

$$-M \cdot (1 - \alpha_j) \le w2_{i,j} \le M \cdot (1 - \alpha_j), \quad i = 1 \ldots NG,\ j = 1 \ldots NXY \tag{5e}$$

$$Q_j + (\lambda - Q_j) \cdot (1 - \alpha_j) - Q_j \sum_{i=1}^{NG} D_{i,j} \cdot w1_{i,j} - (\lambda - Q_j) \sum_{i=1}^{NG} D_{i,j} \cdot w2_{i,j} \le \varepsilon_w + ew_j, \quad j = 1 \ldots NXY \tag{5f}$$

Constraint 5a preserves the sparsity pattern of K given that if $D_{i,jj} \cdot D_{ii,jj}$ is zero the term is zero and this ignored. The basic idea of this approach is taken from the fact that each row of DD^T can be calculated as $DD_i^T = \sum_{jj=1}^{NXY} \times \sum_{ii=1}^{NG} [D_{i,jj} \cdot D_{ii,jj}]$ where it should be noted that constraint 5a does not require DD^T to be computed explicitly as is the case for D^TD (DTD) in the estimability formulations. Additionally, the precision constraints require three free working variables: $w1$ and $w2$ of size NG × NXY and $w3$ of size NG × NXY × NXY where $w3$ is sparse with the identical sparsity pattern of DD^T as determined by $D_{i,jj} \cdot D_{ii,jj}$. This is an improvement of our method over that of Bagajewicz and Cabrera[15] where they require a working variable of size NG × NG × NXY. Although $w3$ working variable is of worst-case size of NG × NXY × NXY, because of the sparsity of K there is a significant working variable reduction even when the additional overhead of $w1$ and $w2$ is considered given that only a small number of $D_{i,jj} \cdot D_{ii,jj}$ are nonzero. Constraints 5b–5e are in fact the linearization of $w1$ given that $w2, w3 = w1 \cdot (1 - \alpha)$. Constraint 5f is the final constraint that determines the diagonal of the covariance yielding the inverse of precision where we assume that the matrix Q is diagonal and Q_j is the a priori sensor variance for variable j if it is measured. It also must be understood that the Q matrix diagonal elements are most likely a relative function of the variable domains meaning that depending on the value of variable its variance or precision is different and hence Q is actually nonlinear though this detail is not explicitly addressed.

In any process plant it is recommended the sensor network in question be a fully observable and redundant system. The rationale for this best practice or guideline is to ensure that all measured variables are observable if its sensor fails and that all unmeasured variables are observable providing complete visibility into the operation of the process at all times. If this is not possible due to high instrumentation and/or sensor lifecycle maintenance costs, there are two alternatives. The first alternative is to admit solutions with nonzero elastic variables (eu_j, ev_j), which indicates that the observability and redundancy constraints were not satisfied hence yielding less visibility and reliability of the sensor network as the trade-off. In this case, different penalty weights can potentially be set for the observability and redundancy constraints depending on what criterion the user or analyst favors most. As a second alternative, the user can exogenously preprocess the process flowsheet to remove less important nodes and/or arcs from it. These deleted nodes and arcs are characterized by a lesser need for granularity because of process reasons. With the preprocessing technique, the total number of variables in the problem decreases, thus potentially decreasing the cost for making the new, preprocessed system fully observable and redundant.

Estimability then Variability Heuristic with Elimination Cuts

Solving any industrial MILP problem to a provably optimal solution can take a very long time especially in the worst case. Fortunately, good integer-feasible solutions can be found early on in the branch-and-bound search process of MILP and these solutions can be considered as practical and useful. Another approach is to use problem-specific heuristics such as those used in production scheduling.[26–28] For large and difficult sensor location problems[§] we propose a prag-

[§] Large sensor location problems constitute systems with several hundred variables. Apart from the sheer size of the problem, other difficulties may be cases where observability- and redundancy-metrics are close to zero, which may be related to the ill-conditioning of the incidence matrices. For nonlinear sensor networks, linearization may constitute another challenge in that for a sensor location problem the user must decide the operating point around which to linearize.

matic but heuristic strategy to find cost optimal measurement placement solutions in reasonable time at acceptable cost.

The idea is to solve the estimability or observability and redundancy problem first then to fix the partition of the *D* matrix into the *A* and *B* incidence matrices for the measured and unmeasured variables respectively and then solve the variability problem second. This is similar to the production scheduling heuristic found in the works of Kelly and Mann[27] and Kelly[29] whereby they solve what is called a "logistics" (quantity-logic) problem first then a "quality" (quantity-quality) problem second when a decomposition of quantity, logic, and quality is required. Our estimability then variability algorithm is as follows:

(1) Solve the estimability MILP problem and retain as many integer-feasible solutions as possible given the allotted amount of time or until global optimality is proved. Apply elimination cuts if available from previous estimability solutions.

(2) Solve the variability LP problem with fixed binary variables for as many times as there are integer-feasible solutions found in Step 1.

(3) If both the estimability and corresponding variability problem solutions have an acceptable amount of elastic or artificial variables then choose the solution with the overall smallest sensor cost and stop.

(4) Else apply what are known as "solution-set," "super-set," and "sub-set" elimination cuts[30] to remove from the search space all or part of the previous integer-feasible solutions of the estimability problem and go back to Step 1.

The basic notion of this heuristic is to use the variability problem as feedback and the estimability problem as feedforward to determine whether the estimability problem has found useful solutions which are variability feasible and suitable. This is similar to the coordinator (estimability) and cooperator (variability) hierarchy structure found in the hierarchical decomposition heuristic.[28] The elimination-set cuts are used at the coordinator level to redirect it to help find integer-feasible solutions which will be cooperator-feasible and the process repeats where for practical problems some compromised or trade-off solution will always exist, i.e., more sensors will need to be added than truly required to respect observability, redundancy, and precision limits. It should also be mentioned that it is possible to reverse the sequence of the heuristic in that solving the variability MILP problem first then the estimability LP problem second with elimination cuts can also be tried. Alternatively, it may also be effective to solve the three aspects individually with the top levels addressing or handling feedback from the bottom levels as elimination-set cuts. For example, a system that respects observability only will have less sensors and hence less cost than a system that simultaneously includes observability and software/hardware redundancy. Therefore, as a heuristic approach, it seems reasonable to solve observability first then fix these measurements then solve redundancy and finally precision. This heuristic is also related to the classical structure of heuristics where they usually include a greedy or constructive search first to find reasonably good solutions quickly then a local or improvement search around a limited neighborhood of these solutions second.

Nonlinear, Dynamic, and Operating-Mode Considerations

For nonlinear problems where the *D* matrix can be substituted with the first-order partial derivative Jacobian matrix of the linearized material, energy, and momentum balances around a predefined operation-point,[27] it is possible to systematically solve several estimability and variability MILP problems for a well represented set of process/operating-condition regions similar to the grid layout proposed by Forbes et al.[31] for real-time optimization point-wise model adequacy validation. From the solutions of these problems it would be possible to make reasonable engineering judgments as to where sensors should be placed in a cost-effective manner notionally respecting the nonlinearities of the underlying process.

For dynamic problems with a uniform or nonuniform discretization of time but externally specified, the *D* matrix can be comprised of many instances of the same static or steady-state *D* matrix where each instance is called a time-slice or time-period. It is possible to determine "collective" observability and redundancy across all time-periods.[32] It is also possible to optimize the entire dynamic *D* matrix although substantially increasing the size and the intractability of the estimability and variability MILP problems.

With regard to operating-modes, it should be evident that when operating the units in different operating-modes or normal-situations, a different set of sensors may be required given that these modes will dictate various disjunctions and discontinuities in the processing, i.e., when producing product *A* units 1 and 2 should be used but when processing product *B* units 2 and 3 should be used. As such, mode-dependent *D* matrices will exist. This may also occur when different abnormal situations or fault scenarios exist or when starting-up or shutting-down a unit. In the case of abnormal situations, the most relevant faults could be enumerated by using one of the many available tools aimed at improving process safety such as HAZOP, signed diagraphs or fault-tree analyses. The methods in this work could be applied to the combination of all fault-dependent *D* matrices in order to indicate the sensor network that yields the safest process configuration. In a dynamic situation (i.e., start-up or shutdown of a unit), besides the fact that the process may behave in a different fashion from normal operation, sensor networks may not be operating within their design regime where some instruments may for instance be outside of their upper or lower range. These situations highlight the need for a special analysis of the sensor network for dynamic cases in order to ensure the process is safe even during these transient operations. To handle both the fault-scenarios and the transient cases it seems prudent to design the sensor network, or more appropriately in this case sensor superstructure, with either multiple *D* matrices simultaneously or sequentially using several *D* matrices separately similar to the nonlinearities and dynamics handling of above.

In the following sections, two illustrative examples are presented that illustrate the new formulations and their application.

Example 1—Simplified Ammonia Network

This case study is a simplified and steady-state ammonia network taken from the work of Carnero et al.,[14] which can

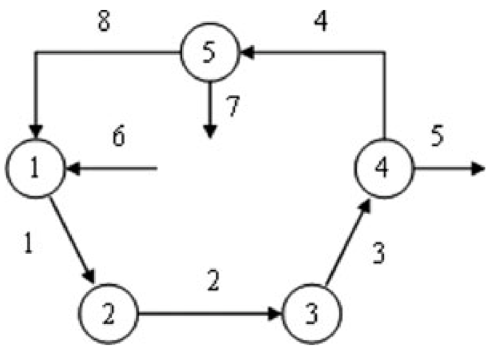

Figure 1. Example 1 (from Carnero et al., 2001).[13]

be seen in Figure 1. The D incidence matrix for this problem is given below:

$$D = \begin{bmatrix} -1 & & & & & 1 & & 1 \\ 1 & -1 & & & & & & \\ & 1 & -1 & & & & & \\ & & 1 & -1 & -1 & & & \\ & & & 1 & & & -1 & -1 \end{bmatrix}$$

All MILP problems in this work are generated and solved using XPRESS-MOSEL version 2.0.0 and XPRESS-MILP version 18.00.01 with all default settings.[33] The penalty costs for all examples were set to the arbitrarily large value of 10^4. When only the observability problem is solved, an overall cost of \$850 is obtained, confirming the results in the work of Carnero et al.[14] where sensors are placed on streams 1, 5, and 7 (Table 1) where this is a nonredundant system with five balance equations and five unmeasured variables. In Table 1, the redundancy- and precision-metrics were calculated after obtaining the sensor location results for enforcing observability.

However, these three measurements are nonredundant (indicated by a zero redundancy-metric) as studied by Carnero et al.[14] If the redundancy requirement for all measured variables is imposed on this problem in addition to the observability requirement, the overall objective cost becomes \$1220 because of the inclusion of a single extra sensor, namely, stream 8 (in bold, Table 2). Therefore, by increasing the cost by \$370 the system becomes incrementally more robust to a single sensor failure because all measured variables are also redundant, i.e., if a sensor fails the measured variable in question can still be estimated (i.e., observed).

In addition to being fully observable and redundant, if the system is also required to satisfy an arbitrary precision tolerance of 0.9 (assuming $\lambda = 1000$ and all $Q_j = 1.0$), the cost increases to \$1570 because an extra stream needs to be measured i.e., stream 2, which is bolded in Table 3. It should be noted that for this case, the MILP problem statistics are: 1338 rows, 328 columns, 3989 nonzero elements, and 16 binary variables. All of the three cases described previously are solved in less than 0.1 CPU seconds on an Intel Pentium processor with 2.13 GHz and 2 GB of RAM.

Table 1. Example 1—Observability Problem

Variables	α_j	Observability-Metric*	Redundancy-Metric*	Precision-Metric*
1	1	–	0	1.00
2	0	1.00	–	1.00
3	0	0.50	–	1.00
4	0	0.33	–	1.99
5	1	–	0	1.00
6	0	0.20	–	1.99
7	1	–	0	1.00
8	0	0.25	–	2.98

*The observability-metric refers to the left-hand side of Eq. 3d, the redundancy-metric refers to the left-hand side of Eq. 4d, and the precision-metric refers to the left-hand side of Eq. 5f.

Table 2. Example 1—Observability and Redundancy Problem

Variables	α_j	Observability-Metric	Redundancy-Metric	Precision-Metric
1	1	–	0.25	0.75
2	0	1.33	–	0.75
3	0	1.00	–	0.75
4	0	1.33	–	1.00
5	1	–	0.25	0.75
6	0	1.00	–	1.00
7	1	–	0.25	0.75
8	***1***	–	0.25	0.75

Example 2—Simplified Olefin Plant

The second example consists of a simplified olefin plant taken from the work Sánchez and Romagnoli[7] and also detailed in Kelly.[1] It contains 29 measured variables, 34 unmeasured variables, and 31 linear, static material balances. In the original problem only five of 34 unmeasured variables are observable indicating that even though $(34 - 5 = 29)$ other unmeasured variables existed in the balance equations their values cannot be estimated. In practice this situation is not recommended as previously mentioned given that if the variables exist in the balance equations they should all be estimable as a general rule-of-thumb. Otherwise if the variables are not relevant to the process in question they should be either removed from the problem altogether or their observability tolerance set to 0 and the elastic variables can be removed. However, it should emphasized that this is not a mathematical requirement given that unobservable and nonredundant variables are handled appropriately in the optimization.

Table 3. Example 1—Observability, Redundancy, and Precision Problem

Variables	α_j	Observability-Metric	Redundancy-Metric	Precision-Metric
1	1	–	1	0.43
2	***1***	–	1.33	0.43
3	0	1.50	–	0.43
4	0	1.50	–	0.86
5	1	–	0.33	0.71
6	0	1.00	–	0.86
7	1	–	0.33	0.71
8	1	–	0.33	0.71

Table 4. Example 2—Observability Problem

Variables	α_j	Observability-Metric	Redundancy-Metric	Precision-Metric	Variables	α_j	Observability-Metric	Redundancy-Metric	Precision-Metric
1	1	–	0.33	2.91	30	0	1.5	–	2.00
2	1	–	0.33	0.20	31	0	1.5	–	4.90
3	1	–	0.83	0.85	***32***	1	–	0	1.00
4	1	–	0.83	0.36	***33***	1	–	0	1.00
5	1	–	1.33	2.43	34	0	2.34	–	1.85
6	1	–	0.5	0.67	***35***	1	–	0	1.00
7	1	–	1	0.57	36	0	1.25	–	0.58
8	1	–	1	2.57	37	0	0.83	–	0.18
9	1	–	1.2	0.17	38	0	0.83	–	0.13
10	1	–	1.2	0.61	39	0	1.25	–	0.03
11	1	–	1.2	0.51	40	0	1.06	–	1.34
12	1	–	1.2	0.02	***41***	1	–	0	1.00
13	1	–	1	0.06	***42***	1	–	0	1.00
14	1	–	1.2	0.05	43	0	1.06	–	1.99
15	1	–	0.2	0.01	44	0	0.57	–	2.98
16	1	–	1.2	0.00	***45***	1	–	0	1.00
17	1	–	1.2	0.02	46	0	0.4	–	4.97
18	1	–	1.2	0.09	***47***	1	–	0	1.00
19	1	–	1.2	0.01	***48***	1	–	0	1.00
20	1	–	1	0.25	***49***	1	–	0	1.00
21	1	–	1.06	0.34	50	0	1.06	–	1.00
22	1	–	1.06	0.02	51	0	0.28	–	4.97
23	1	–	2	0.27	52	0	0.33	–	1.40
24	1	–	1.06	0.01	53	0	0.4	–	0.40
25	1	–	1.06	0.25	54	0	0.26	–	2.34
26	1	–	1.06	0.13	55	0	1.06	–	1.12
27	1	–	0.06	0.09	56	0	1.06	–	1.40
28	1	–	0.06	0.12	57	0	1.06	–	1.00
29	1	–	0.06	0.40	***58***	1	–	0	1.00
					59	0	0.24	–	2.98
					60	1	–	0	1.00
					61	0	0.24	–	1.99
					62	0	0.24	–	2.98
					63	0	1.06	–	2.00

To correct the lack of observability in this problem the 29 original measured variables are fixed ($\alpha = 1$) and an upper bound of 20 extra sensors is placed on the retrofit problem as follows:

$$\sum_{j=30}^{NXY} \alpha_j \leq 20 \tag{6}$$

Additionally, all sensors are arbitrarily assumed to have an equal cost of \$1 because no sensor cost information is available from the original authors of the example. For calculating the precision-metric, the measurement variances for variables 1–29 are taken from the work of Sánchez and Romagnoli,[7] whereas the remaining hypothetical sensor variances are assumed to be at unity, i.e., $Q_j = 1$. The value of λ was set at 2300 according to the procedure outlined by Kelly.[1] The observability only MILP problem consisted of 23,564 rows, 4095 columns, 93,500 nonzero elements, and 63 binary variables. The first solution of \$125.0 is found in 11 nodes at 2 CPU seconds, with an integrality gap of 76.8%. At 34 nodes and 3 CPU seconds a solution of \$40.0 is found with an integrality gap of 27.5%. The optimization problem is allowed to run for up to 1000 CPU seconds at which time the results in Table 4 are obtained with an integrality gap of 7.5%. It is worth mentioning that 3481 integer-feasible solutions are found during the course of the branch-and-bound search, a very large portion of which had the same objective function value as the final solution of \$40.0, indicating a highly degenerate problem which is expected because of its inherent correlation structure.

This retrofit problem is initially solved with only observability constraints. Even so, comparing the new precision-metrics in Table 4 with the ones from the original problem with 29 measurements in Table 5, it is clear that because of the full observability of variables in the retrofit case the precision of the unmeasured variables increased significantly as a byproduct or effect of the estimability specifications.

From Table 4, one can see that all unmeasured variables are observable but the 11 extra measured variables (in bold) are nonredundant (because their redundancy-metric is equal to 0). Following the decomposition heuristic suggested in the previous section, all (29 + 11 = 40) sensors are fixed in order to solve the redundancy problem. These results can be seen in Table 6.

The redundancy problem contains 47,126 rows, 8001 columns, 194,316 nonzero elements, and 126 binary variables. The first solution (\$46) is found in 41 nodes with a gap of 13.04% at 4 CPU seconds, while the last of 385 integer-feasible solutions (\$46) is found in 1454 nodes with a gap of 2.17% at 72 CPU seconds. In total, six extra sensors are added to the system in order to make it fully redundant (bold

Table 5. Example 2—Precision-Metric for Original Problem

Variable	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
Precision-Metric	2.91	0.20	0.85	0.36	2.43	0.67	0.57	2.57	0.17	0.61	0.51	0.02	0.06	0.05	0.01	0.00
Variable	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32
Precision-Metric	0.02	0.09	0.01	0.25	0.34	0.02	0.27	0.01	0.25	0.13	0.09	0.12	0.40	920.47	921.05	1380.12
Variable	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48
Precision-Metric	1380.12	1150.21	1150.21	0.58	0.18	0.13	0.03	621.43	621.42	820.31	749.81	550.79	545.61	1429.57	1429.57	1008.13
Variable	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	
Precision-Metric	806.38	806.38	971.61	545.65	0.40	812.92	687.60	766.85	766.71	766.71	872.91	687.58	665.59	550.79	916.54	

variables 31, 34, 46, and 54). The remaining two sensors are placed on the variables with zero redundancy-metric (indicated by asterisks in Table 6), thus making them hardware-redundant ($\beta = 1$).

In practice it would be reasonable to stop the heuristic at this point if desired because all variables in the system are estimable. If in addition a precision tolerance is required, another optimization problem can be solved where that value must be enforced or respected. In this case, the tolerance is arbitrarily set to a value of 1.7 for all measured and unmeasured variables. The results of fixing the previous measurements and solving the precision problem are provided in Table 7.

This problem contains 39,061 rows, 11,340 columns, 114,690 nonzero elements, and 63 binary variables. The final solution ($46) is found in six nodes with a gap of 2.7% at 4 CPU seconds. Note that the precision constraint was indeed respected by all variables that previously exceeded the precision tolerance (cf. variables 8, 51, and 63). This was achieved by adding two new sensors on variables 30 and 63 (in bold) which then only requires one hardware redundancy specification on variable 58 in order to satisfy the full redun-

Table 6. Example 2—Redundancy Problem

Variables	α_j	Observability-Metric	Redundancy-Metric	Precision-Metric	Variables	α_j	Observability-Metric	Redundancy-Metric	Precision-Metric
1	1	–	0.5	1.46	30	0	2	–	1.31
2	1	–	1	0.20	31	***1***	–	1.5	0.83
3	1	–	2	0.58	32	1	–	1.5	0.83
4	1	–	2	0.33	33	1	–	1.5	0.83
5	1	–	2	1.55	34	***1***	–	2	0.65
6	1	–	1	0.52	35	1	–	2	0.65
7	1	–	1	0.56	36	0	1.25	–	0.58
8	1	–	1	1.89	37	0	0.833	–	0.18
9	1	–	1.2	0.17	38	0	0.833	–	0.13
10	1	–	1.2	0.61	39	0	1.25	–	0.03
11	1	–	1.2	0.51	40	0	1.142	–	1.10
12	1	–	1.2	0.02	41	1	–	0.458333	0.82
13	1	–	1	0.06	42	1	–	0.458333	0.82
14	1	–	1.2	0.05	43	0	1.5	–	1.30
15	1	–	0.2	0.01	44	0	1.5	–	1.42
16	1	–	1.2	0.00	45	1	–	0.5	0.61
17	1	–	1.2	0.02	46	***1***	–	0.458333	0.82
18	1	–	1.2	0.09	47	1	–	0.458333	0.82
19	1	–	1.2	0.01	48	1	–	0.458333	0.82
20	1	–	1	0.24	49	1	–	***0****	1.00
21	1	–	1.125	0.33	50	0	1.142	–	1.00
22	1	–	1.125	0.02	51	0	0.666	–	2.29
23	1	–	2	0.27	52	0	0.75	–	0.82
24	1	–	1.125	0.01	53	0	0.666	–	0.37
25	1	–	1.125	0.25	54	***1***	–	0.291667	0.69
26	1	–	1.125	0.13	55	0	1.2	–	0.78
27	1	–	0.125	0.08	56	0	1.2	–	1.37
28	1	–	0.166667	0.12	57	0	1.2	–	1.00
29	1	–	0.166667	0.37	58	1	–	***0****	1.00
					59	0	0.666	–	1.46
					60	1	–	0.291667	0.69
					61	0	0.533	–	1.19
					62	0	0.5	–	1.42
					63	0	1.142	–	1.82

Table 7. Example 2—Precision Problem

Variables	α_j	Observability-Metric	Redundancy-Metric	Precision-Metric
1	1	–	1	1.05
2	1	–	1	0.20
3	1	–	2	0.58
4	1	–	2	0.33
5	1	–	2	1.29
6	1	–	1	0.51
7	1	–	1	0.56
8	1	–	1	1.69
9	1	–	1.2	0.17
10	1	–	1.2	0.61
11	1	–	1.2	0.51
12	1	–	1.2	0.02
13	1	–	1	0.06
14	1	–	1.2	0.05
15	1	–	0.2	0.01
16	1	–	1.2	0.00
17	1	–	1.2	0.02
18	1	–	1.2	0.09
19	1	–	1.2	0.01
20	1	–	1	0.24
21	1	–	1.14286	0.33
22	1	–	1.14286	0.02
23	1	–	2	0.27
24	1	–	1.14286	0.01
25	1	–	1.14286	0.25
26	1	–	1.14286	0.13
27	1	–	0.142857	0.08
28	1	–	0.166667	0.12
29	1	–	0.166667	0.37
30	***1***	–	2	0.57
31	1	–	2	0.78
32	1	–	2	0.64
33	1	–	2	0.64
34	1	–	2	0.64
35	1	–	2	0.64
36	0	1.25	–	0.58
37	0	0.833333	–	0.18
38	0	0.833333	–	0.13
39	0	1.25	–	0.03
40	0	1.16667	–	1.08
41	1	–	0.47619	0.81
42	1	–	0.47619	0.81
43	0	1.5	–	1.25
44	0	1.5	–	1.34
45	1	–	0.5	0.61
46	1	–	0.47619	0.81
47	1	–	0.47619	0.81
48	1	–	1.33333	0.58
49	1	–	1.14286	0.65
50	0	1.16667	–	0.65
51	0	0.7	–	1.65
52	0	0.75	–	0.82
53	0	0.666667	–	0.37
54	1	–	0.309524	0.68
55	0	1.2	–	0.78
56	0	1.2	–	1.37
57	0	1.2	–	1.00
58	1	–	***0****	1.00
59	0	0.7	–	1.44
60	1	–	0.309524	0.68
61	0	0.583333	–	1.16
62	0	0.583333	–	1.34
63	***1***	–	1.14286	0.65

dancy restrictions. It should also be highlighted that variable 51 does not require a sensor in order to satisfy the precision constraint. Moreover, this improved formulation required [1953 ($w1$) + 1953 ($w2$) + 7308 ($w3$) = 11,214] working variables, whereas the method of Bagajewicz and Cabrera[15] would require ($31 \times 31 \times 63 = 60{,}543$) working variables in order to represent the dense inverse of their kernel matrix resulting in a [$(60{,}543 - 11{,}214)/60{,}543 \times 100 = 81.5\%$] reduction in the number of working variables.

Conclusions

Presented in this work are the details of mathematically modeling observability, software/hardware redundancy, and the diagonals of the covariance matrix of both the measured and unmeasured variables in error-in-variables type of statistical optimization problems. All three salient aspects of the sensor location problem are explicitly and analytically formulated in MILP constructs where the observability and redundancy constraints are new and are based on the well-known Schur complement. An improved formulation from the work of Bagajewicz and Cabrera[15] is provided for optimizing precision which takes advantage of the kernel matrix sparsity found in the reconciliation and regression regularization technique of Kelly.[1] The methods are demonstrated through two illustrative examples from the literature. Considerations for nonlinearities, dynamics, modes of operation including abnormal-situations, and the intractability of industrial-sized MILP problems are also offered.

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Appendix: Summary of Relevant Aspects of Previous Work[1]

This appendix highlights the aspects from the work of Kelly[1] that are relevant to the understanding of this article. The general linear data reconciliation problem can be represented as follows:

$$\begin{aligned} \min_{x} \quad & J = (x_m - x)^T Q^{-1} (x_m - x) = x_a^T Q^{-1} x_a \\ \text{s.t} \quad & f = Ax + By + Cz = 0 \end{aligned} \tag{A1}$$

In Eq. A1, x_m, x_a, and x correspond to the measurements, adjustments, and reconciled variables, respectively, Q is the measurement variance-covariance matrix, and y and z are unmeasured and fixed variables, respectively. By using the method of Lagrange multipliers for the linear data reconciliation problem, it is well known that the solution to the above data reconciliation problem may be obtained through the equations below. However, the equation for y is derived similarly as the equation for x when all ys are assumed to have same large variance denoted as λ. Kelly also presents the method for the general nonlinear data reconciliation case, which is not shown here for conciseness purposes.

$$x = x_m - QA^T K^{-1}(Ax_m + Cz) \tag{A2}$$

$$y = \lambda B^T K^{-1}(Ax_m + Cz) \tag{A3}$$

In Eqs. A2 and A3, K is the kernel matrix which is expressed as

$$K = AQA^T + \lambda BB^T \tag{A4}$$

In Eqs. A2–A4, λ is a regularization or ridge-regression parameter, which as mentioned, represents the large equal variance estimate for all unmeasured variables. Kelly[1] presents a guideline for determining the value for this parameter in his appendix based on the terminal rank of the kernel matrix for varying λs.

Following Kelly,[1] to perform the measured and unmeasured variable classification, it is necessary to partition the B matrix into dependent and independent columns as follows:

$$B = [B_{12} \quad B_{34}] \tag{A5}$$

where B_{12} and B_{34} correspond to the independent and dependent columns of B, respectively. Kelly[23] presents an efficient method based on the Schur complement to determine dependent columns of a matrix automatically by successively adding one column at a time of the original B matrix to the problem. Once B_{12} and B_{34} have been obtained by using the method(s) outlined in the work of Kelly,[23] the observability of unmeasured variables and the redundancy of measured variables can be determined by the following found in that of Kelly[1]:

$$S_o = [B_{12}^T \quad B_{12}]^{-1} B_{12}^T B_{34} \tag{A6}$$

$$\begin{aligned} s_R &= \text{diag}\{A^T(I_g - B_{12}(B_{12}^T \quad B_{12})^{-1}B_{12}^T)A\} \\ &= \text{diag}\{A^T E A\} \end{aligned} \tag{A7}$$

In A6, if any row of S_o contains any nonzero elements, the corresponding variable is deemed to be nonobservable where by default all columns of B found in B_{34} are unobservable. In A7, if any value of s_R is equal to zero, the corresponding variable is deemed to be nonredundant.

Manuscript received Nov. 12, 2007, and revision received Jan. 31, 2008.