Optimal Selection of Measuring Points in Complex Plants by Linear Models

František Madron and Vladimír Veverka
System Engineering Dept., Research Institute of Inorganic Chemistry, 400 60 Ústí nad Labem, Czechoslovakia

For reliable information on operating plants it is essential to design measuring points well by selecting directly measured quantities from the set of all measurable quantities.

This article deals with a new method for optimizing measurement design. It is based on multiple Gauss-Jordan elimination of the system of linear mathematical model equations and solves the problem of instrumentation design in new plants as well as the problem of optimizing existing measuring systems. Optimization methods for linear objective functions and for objective functions of general type are proposed. The method also offers a complex classification of quantities (observability and redundancy). After the optimization, the problem is presolved and is ready for an optimal processing of measured data. The mathematical model is reduced to the minimum set of equations and quantities relevant to the solution of a given problem. From a numerical standpoint, the solution is efficient.

Introduction

The analysis of data measured in operating plants, which is essential for control, optimization, mathematical parameters estimation, depends strongly on the *measurement planning* (*measurement design*). Measurement design is a multilevel problem, ranging from details of measurement to a global measurement strategy. Of these levels, the selection of directly measured quantities is probably the most important. This activity, also called *measurement placement* (Stanley and Mah, 1981), plays an important role in the design of instrumentation in new plants as well as in the planning of studies carried out in operating plants in the course of optimization, retrofitting or debottlenecking.

The problem of design of measuring points in chemical engineering literature is not new, though in many previous works the optimization aspect is not explicitly stated. Measurement placement is closely connected with the problem of quantities classification.

The classification of quantities according to their redundancy or observability (see Figure 1) is particularly important in measurement planning (selection of directly measured quantities) and in the identification of mathematical models by statistical processing of measured data.

The classification was developed mainly for use in the balancing complex plants in process industries. The methods developed are based on the solvability analysis of sets of balance equations (Václavek et al., 1972; Crowe, 1989) and on the analysis of a structure of balanced system (Václavek and Loučka, 1976; Václavek and Vosolsobě, 1981; Madron and Výborný, 1983). A series of systematic research by Mah and his coworkers in this area is summarized in a monograph (Mah, 1990), where also a comprehensive survey of the state of the art of classification can be found.

Problem Statement

Let us consider the set P of quantities (variables) occurring in a given problem. The set consists of two subsets:

P_1 = measured quantities (for example, by an existing instrumentation in a given plant. If we design completely new instrumentation, P_1 is an empty set.)

P_2 = unmeasured quantities

The sets P_1 and P_2 are disjoint and their union is the set P.

Let us limit ourselves to the case when the quantities P are subject to K linear equations (constraints) constituting what is called a *general linear model*:

$$\mathbf{By} + \mathbf{Ax} + \mathbf{c} = \mathbf{O}. \tag{1}$$

where

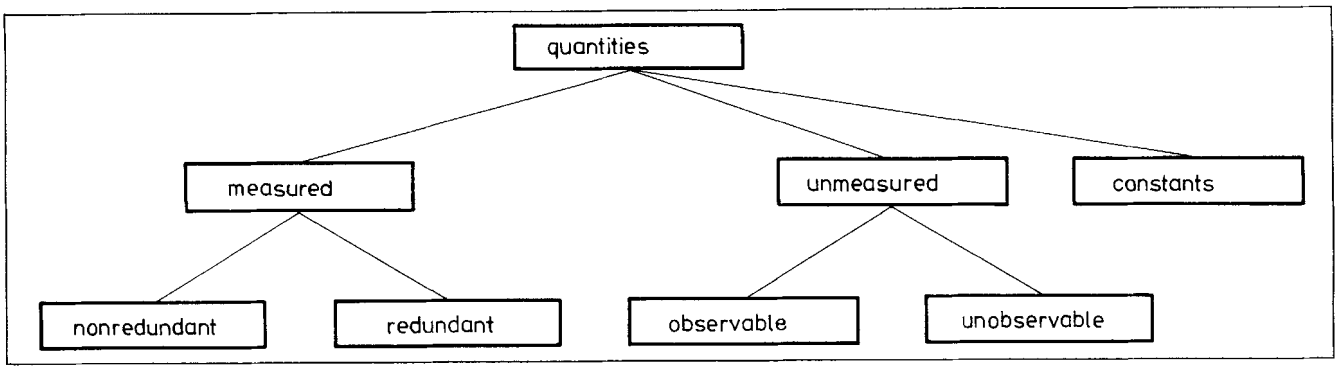

Figure 1. Classification of quantities.

x = vector of directly measured quantities
y = vector of directly unmeasured quantities
A, B, c = constant matrices and column vector

Let us further define two other subsets of the set P:

P_3 = quantities whose values have to be known (*required quantities*)
P_4 = quantities whose values are not required

The latter two subsets are again disjoint, and their union is P.

We now put the following questions:

1. Are the equations independent? If not, what is the maximal set of independent equations?
2. Does the system (Eq. 1) contain contradictory equations?
3. Are all of the required unmeasured quantities determinable (observable)? If not, which quantities are indeterminable (nonobservable)? Which unmeasured quantities have to be measured in addition to determine all required unmeasured quantities?
4. Which directly measured quantities are just determined and which are redundant and thus adjustable? How can the choice of the additional measurements be optimized?
5. Are there measured quantities and equations present that do not contribute to the determination of the required quantities? How can one find the minimal set of equations that comprises all information concerning the required quantities?
6. How can the overall complex of data processing (reconciliation of redundant data, detection and identification of gross errors, and so on) be organized in an optimum way?

This problem statement is an extension of that of Václavek et al. (1972).

Before answering these questions, let us formulate objective functions that will be further used in the optimization of measurement design.

Objective Functions

The simplest is the case of linear objective function. Let us consider the case in which we intend to minimize the overall cost of measurement. The objective function Φ is of the form:

$$\Phi = \sum_{i=1}^{I_m} c_i \tag{2}$$

where

I_m = number of measured quantities
c_i = costs belonging to ith measurement

The costs may represent, for example, the investment needed to install new instrumentation, the cost of regular maintenance, or the average expenses connected with performance of instrumentation in some time interval. Let us realize that the cost may be zero if the instrument is already installed. Let us note that the objective function is a simple linear function of measurement costs, the coefficients being 0 or 1.

In some cases, we try to avoid the measurement of some quantities that are not easy to measure. Usually it is difficult to express *measurability* quantitatively. Nevertheless, we are often able to order quantities in the sense of increasing measurability. If we now select, using a method described below, certain quantities as unmeasured (therefore computed from the constraints), our goal is to make the selection such that we minimize the objective function (Eq. 2) where c_i is the ordinal of the not-to-be-measured quantities (in number I_m). Indeed, the lower is the sum of these ordinals, the more preferred are the hard-to-measure quantities if qualified as unmeasured.

Another point to be respected in measurement design is the precision of results. As an example, consider the objective function representing mean square error of the result:

$$\Phi = \left[\sum_{i=1}^{I_r} \sigma_i^2 / I_r \right]^{1/2} \tag{3}$$

where

σ_i = standard deviation of ith required quantity (measured directly or calculated)
I_r = number of required quantities

It is important to realize here that the standard deviation σ_i itself is (due to possible reconciliation) complex functions of the selection of directly measured quantities and of their precision (standard deviations). The objective function (Eq. 3) is thus strongly nonlinear.

Theory

The intuitive concepts of observability (of unmeasured variables) and redundancy (of measured ones) are explained in the literature.

For example, according to Kretsovalis and Mah (1988): "If a subset of constraint equations is solvable with respect to the unmeasured variables occurring in it, then these quantities are said to be *observable*.... If we can delete a measurement

without making the associated variable unobservable, then the measurement is said to be *redundant*."

It is difficult to translate these verbal formulations into a precise mathematical language for the general case (see Stanley and Mah, 1981). In the case of linear constraints (Eq. 1), a precise algebraic classification is possible; see Appendix A where the classification is related to the proposed method of solution. (The Appendix is written for mathematically oriented readers; thus, those who are not interested in formal precision and proofs may use an intuitive interpretation following directly from the explicit description of the method. We also use "determinable" instead of "observable.")

The interpretation of observability appears to be unambiguous. The classification is purely algebraic and has nothing to do with statistics. In practice, the formally *nonredundant* variables are frequently considered *nonadjustable*, that is, they are not adjusted during data reconciliation, changing their values does not improve the statistical criterion for reconciliation, and the measured values remain thus nonadjusted.

This often accepted assumption, however, holds true only in the (frequent) case of a *diagonal* covariance matrix (uncorrelated measuring errors). The notion of nonredundancy and nonadjustability coincides; but this is not the case when the covariance matrix is not diagonal (Crowe, 1989, p. 2914). The conclusions drawn here concerning observability will be of *general character*, whereas comments concerning adjustment of measured values (reconciliation) are limited to the most common case of a *diagonal covariance matrix of measuring errors*.

Solution of the Problem

Let us now solve the problem stated above systematically. We shall focus our attention to the linear model (Eq. 1).

First, we set up the extended matrix from the matrices $\boldsymbol{B}$, $\boldsymbol{A}$ and vector $\boldsymbol{c}$ occurring in the model (Eq. 1), see Figure 2. We assume that the variables (columns of matrices $\boldsymbol{B}$ and $\boldsymbol{A}$) have been arranged into groups forming submatrices according to whether the values are or are not required. Further, we have separately ordered the columns of both submatrices of $\boldsymbol{B}$ (unmeasured variables) according to their measurability; the relatively easily measurable variables are on the right sides.

To the initial macromatrix arranged in this manner we shall

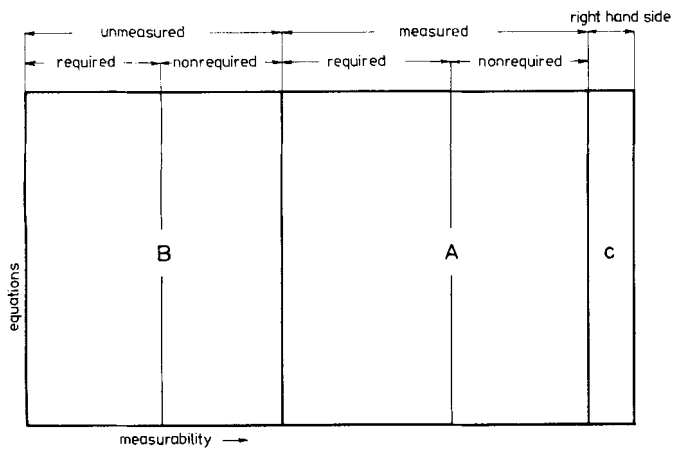

Figure 2. Macromatrix formed by matrices *B*, *A* and vector *c*.

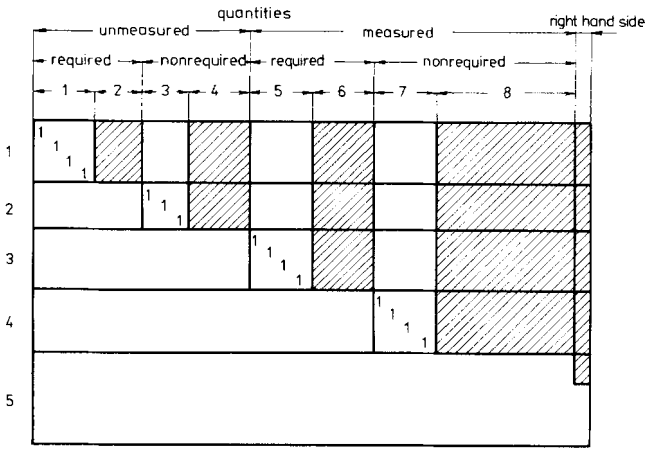

Figure 3. Macromatrix from Figure 2 after Gauss-Jordan elimination.

□, zero element; ⧈, unit element, ▨, general element.

now apply Gauss-Jordan elimination. The procedure is shown in Figure 3.

In elimination, the pivots are first used from the submatrix corresponding to unmeasured required values. When possible, in any successive step we use a pivot in the column following only the prescribed order (if an arbitrary order is used in the submatrix, the columns could be mixed and some easy-to-measure variables would become the hard-to-measure ones). A permutation of columns of the submatrix is admitted only if there are only zero elements in the subsequent column under the row of the last pivot. Such a column is then placed at the end of the submatrix of unmeasured required variables and is replaced by its next right neighbor. After such elimination, one obtains a unit submatrix in the left upper corner and a general submatrix on its right side. The submatrices will further be denoted as $\boldsymbol{Z}_{1,1}$ and $\boldsymbol{Z}_{1,2}$, as shown in Figure 3. Below these submatrices are zeros only. The submatrix $\boldsymbol{Z}_{1,2}$ may also not be present.

The elimination succeeds using the pivots from the submatrix of unmeasured nonrequired variables in an analogous way. One, thus, obtains unit submatrix $\boldsymbol{Z}_{2,3}$, zero submatrix $\boldsymbol{Z}_{1,3}$, and general submatrices $\boldsymbol{Z}_{1,4}$ and $\boldsymbol{Z}_{2,4}$.

Further elimination steps can be followed similarly with pivots from the submatrices corresponding to measured required and measured nonrequired quantities, respectively. Here, we are free in using pivots from the whole respective submatrices because the effect of mixing is irrelevant. Pivoting can be oriented toward improving numerics of elimination algorithm (selecting a pivot with the greatest absolute value) or toward minimizing filling-in of matrices that are generally sparse. The general format of the macromatrix after all elimination steps is shown in Figure 3.

In addition, we try to find certain submatrices (when they exist), as shown in Figure 4.

1. If in submatrices $\boldsymbol{Z}_{1,2}$ and $\boldsymbol{Z}_{1,4}$, there exist some zero rows simultaneously, the rows are reordered to obtain zero submatrices $\boldsymbol{Z}_{1a,2}$ and $\boldsymbol{Z}_{1a,4}$. We thus modify the initially unit submatrix $\boldsymbol{Z}_{1,1}$. We then can reorder the columns in the vertical band 1 to regenerate the unit submatrix.

2. In the submatrix $\boldsymbol{Z}_{1b,4}$ we try to find zero columns and form thus submatrix $\boldsymbol{Z}_{1b,4a}$.

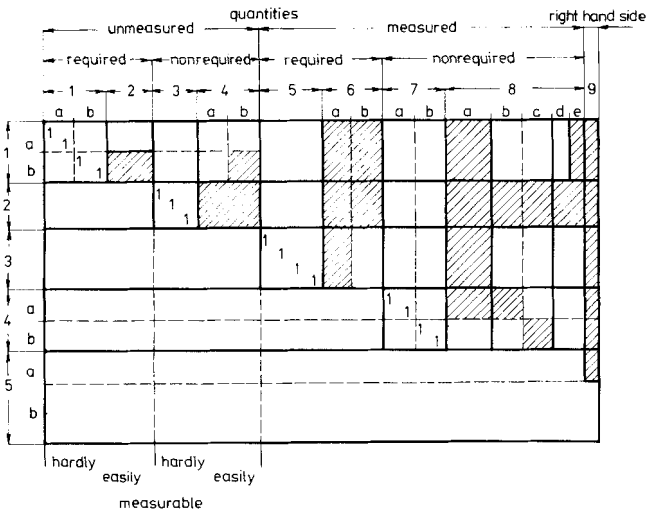

Figure 4. Macromatrix from Figure 3 after formation of zero submatrices.

3. If there are zero columns in the matrix $Z_{3,6}$, they will form zero submatrix $Z_{3,6b}$.

4. If there exist simultaneously zero columns in the matrices $Z_{3,8}$ and $Z_{4,8}$, they will form submatrices $Z_{3,8de}$ and $Z_{4,8de}$ (the double index *de* will be explained below).

5. If there are zero columns in the submatrix $Z_{1,8de}$, they will form submatrix $Z_{1,8d}$.

6. If there exist zero columns simultaneously in the matrices $Z_{1,8}$ and $Z_{3,8}$ in addition to vertical bands 8*d*, they will form zero submatrices $Z_{1,8bc}$ and $Z_{3,8bc}$ (see below for the subdivision into *b* and *c*).

7. Finally, by permutations of rows and of columns we try to rearrange the matrix $Z_{4,8abc}$ into the form shown in Figure 4. Here, one has to obey the rule that the right upper zero submatrix can arise only from the columns of the submatrices $Z_{4,8bc}$; otherwise, the zero submatrices formed according to point 6 above would be destroyed. A procedure leading to such an arrangement (if it exists) is described in Appendix B.

Results

We can now answer the questions posed in the Problem Statement section.

1. The equations are dependent on one another, if and only if in the macromatrix after elimination (Figure 3), there are zero rows. We thus eliminated equations that are linear combinations of the others.

2. The system contains contradictory equations (that cannot be satisfied even if the measured values have been reconciled), only when the subvector $Z_{5,9}$ contains at least one nonzero component. We then have a contradiction of the type 0 = nonzero constant. Such discrepancy has to be made clear and removed.

3. All required unmeasured quantities are determinable (observable), if and only if after the elimination, the submatrices $Z_{1b,2}$ and $Z_{1b,4b}$ are absent. In the opposite case, indeterminable (nonobservable) required quantities are present; they are just those corresponding to the vertical bands 1*b* and 2. To make all required quantities determinable, certain quantities have to be measured in addition; we choose those corresponding to columns 2 and 4*b*. This choice is warranted by the fact that we have ordered the quantities according to their measurability; we have thus preferred the more easily measurable ones. See Appendix C for a theoretical discussion.

4. Quantities (nonredundant), which has been just determined, correspond to columns with zero elements in all rows 3 and 4 (see Appendix A). They are thus represented by columns 6*b* and 8*de*; other measured quantities are redundant (adjustable).

5. The suggested procedure has automatically eliminated all dependent equations. In addition, one can disregard the equations corresponding to the horizontal band 2, which concerns only nonrequired, unmeasured quantities. Further, the horizontal band 4*b* contains equations in certain nonrequired, measured variables only (columns 7 and 8*c*); the reconciliation of the corresponding measured values is not necessary, because it does not interfere with the reconciliation of the required, measured values and because they are needed only for the computation of nonrequired, unmeasured quantities via submatrix $Z_{2,8c}$. (Observe that this conclusion is based on the assumption that the covariance matrix is diagonal.) Also the equations 4*b* can thus be eliminated. Once it is achieved, we can discard the variables corresponding to vertical bands 3,4*a* (see point 3 above) and 7*b*, 8*cd*. The linear system of constraints reduced in this manner contains all of the information contained in the initial system, regarding the required quantities. The reduced system is in Figure 5. Here, we assume that the necessary additional measurements have been carried out as suggested.

6. The procedure enables one to set up a new system that can be solved in a simple way. Without problems, one can eliminate the dependent equations; it is further necessary to measure certain additional, but so far unmeasured, quantities. Then, the requirements for the independence of equations and parameters determinability are fulfilled. Further reduction is basically not necessary. If, however, the above described elimination process has been realized completely, further solution is considerably facilitated.

First, one has to carry out the additional measurements. The quantities will correspond to the vertical bands 2 and 4*b*. These quantities are then measured nonadjustable; in Figure 5, they are placed at the end of the matrix.

The system has been decomposed into two subsystems. The equations corresponding to horizontal bands 3 and 4*a* contain only measured quantities and are used for the reconciliation of adjustable quantities. It is a reconciliation of directly measured quantities with a set of constraints (see, for example, Mah, 1990, p. 388).

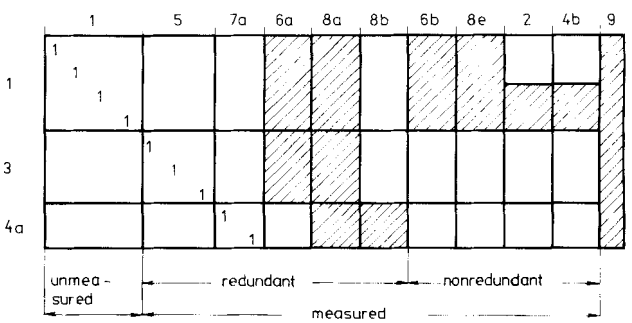

Figure 5. Reduced macromatrix from Figure 4.

After the reconcilation is effected, adjusted values are substituted into equations of the horizontal band 1, and the unmeasured values (vertical band 1) are simply computed. Similarly, a complex processing of the measured data (propagation of random errors, detection of gross errors, and so on) can be realized (see Madron, 1991, for example).

Measured data inconsistency is analyzed using the equations from bands 3 and 4*a* only. The remaining equations contain no information in this respect.

Let us finally remark that if the covariance matrix of measured values happens to be nondiagonal, the detailed rearrangements of columns 5–8 in Figure 3 to the form in Figure 4 are needless. We then have to use the whole nonreduced submatrix of horizontal bands 3 and 4 for reconciliation.

Optimality of the Solution

Let us limit ourselves, at the beginning, to the linear objective function (Eq. 2). The detailed discussion of this case is presented in Appendix C. It is shown there that the solution is the optimum one [with the minimum value of function (Eq. 2)], with the exception that there are some nonobservable, nonrequired quantities present. In this case, the optimality of the solution is not warranted, even if the method looks like good heuristics. In this context, the solution does not represent a global optimum, but only a good, feasible solution applicable to the solution of practical problems.

Much more difficult is the situation in the case of a nonlinear objective function of the type (Eq. 3). Numerous case studies have shown that the optimum solution according to the objective function (Eq. 2), that is, optimization as the cost of the measurement concerns, yields the solution that is unacceptable from the viewpoint of the precision of results. It means that the solution with minimum costs is the solution with some unmeasured quantities at the same time, which are theoretically observable, but with unacceptably low precision (for example, the confidence interval wider than the value of the quantity). In this case, the following optimization method can be recommended. The method is analogous to the direct search in graphs that proved efficient for optimization of measurement designs in single-component mass balancing (Madron and Výborný, 1983).

For the two measurement designs with the same number of measured quantities, let us define their *distance* as the number of distinct measured quantities between these two designs. The designs of distance one differ only in one measured quantity (one measured quantity in one design is replaced by one unmeasured quantity in the other design).

Optimizing the measurement design with Figure 5 is straightforward. We are supposed to start from a suboptimal base design, for example, by the method described in the preceding paragraph. All measurement designs of distance one from the base design can be found easily by exchanging quantities (columns) of macromatrix in Figure 5. The quantities from the vertical band 1*b* (see Figure 4) are exchanged with quantities in vertical bands 2 and 4*b*. The number of all designs of distance one equals that of nonzero entries in matrices $Z_{1,2}$ and $Z_{1,4b}$. The objective function is evaluated for all designs of distance one, and the design with the minimum value of the objective function is exchanged with the base design. The optimization is continued until a local optimum is found (there is no better design in the distance one of the last design).

The proposed optimization algorithm enables one to find the local optimum of a general objective function. The evaluation of objective functions requires only a modest amount of computation (in the essence the multiplication of matrices $Z_{1,2}$ and $Z_{1,4b}$ by vectors of variances of measured quantities). Even problems of realistic dimensionality can be solved efficiently on personal computers.

The algorithm does not guarantee finding of global optimum (at least we have not been successful in proving that). It should be noted that there exists a method of finding the global optimum, that is based on enumeration of all possible measurement designs. Let us form a matrix Z_c composed of submatrices $Z_{1,1}$, $Z_{1,2}$ and $Z_{1,4b}$. The number of all possible designs equals

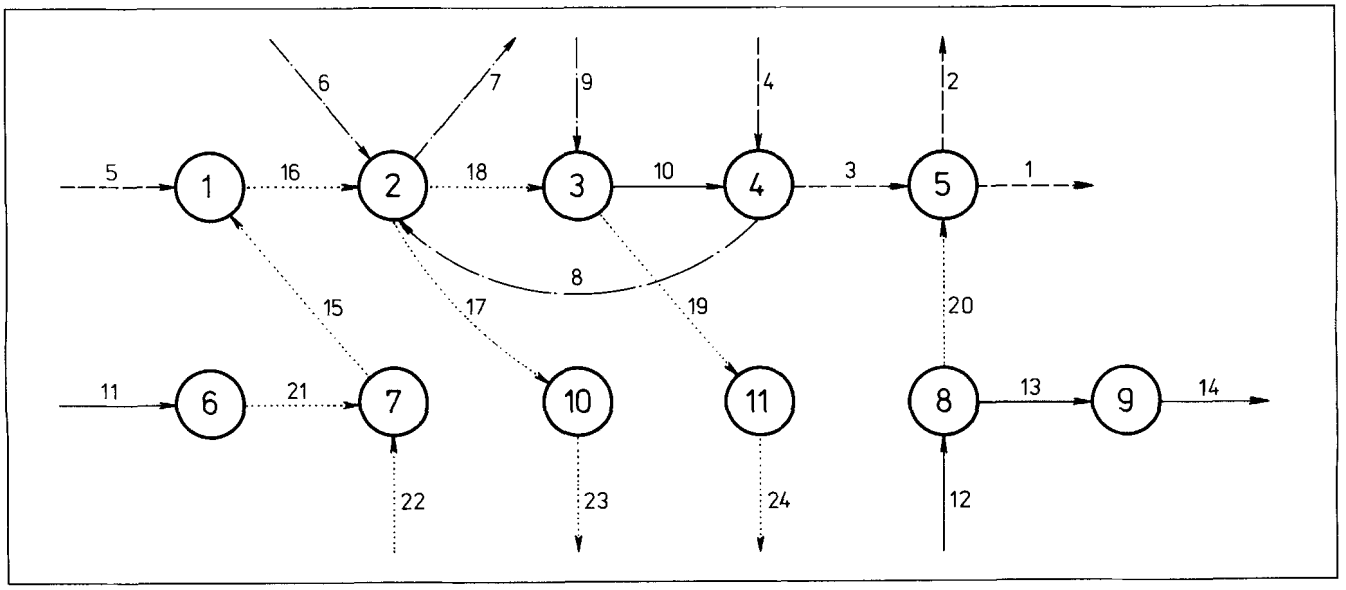

Figure 6. Balance scheme.

—, measured required; ...., measured nonrequired; - - - -, unmeasured required; — • —, unmeasured nonrequired.

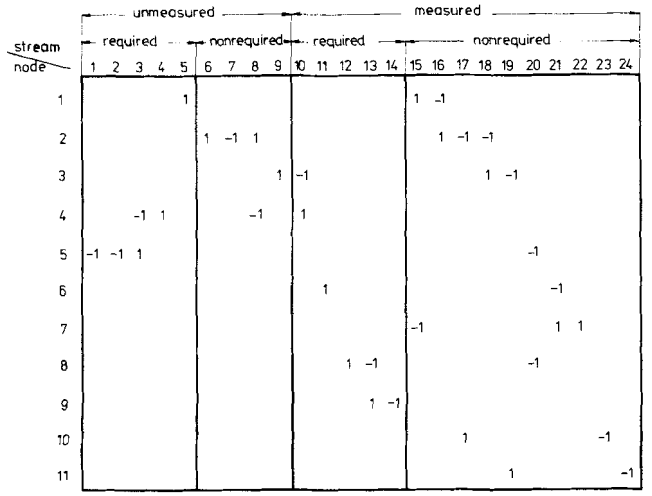

Figure 7. Mathematical model of mass balance (example).

that of all regular matrices that can be formed by selecting columns of the matrix Z_c. This task has been already solved during an analysis of electrical networks. The solution (enumeration of all regular submatrices of a matrix) is explained by, for example, Chen (1971, p. 365). However, the number of all possible measurement designs (number of all regular submatrices of a matrix) is prohibitive in real problems as this number can reach billions even in modest industrial problems (Madron, 1991).

Example

The procedure described above will be demonstrated by an example of mass (single-component) balance. In this case, the matrices A and B represent so-called incidence matrices of measured and unmeasured streams, respectively. The element of incidence matrice on ith row and jth column equals 1, -1, or 0 if jth stream enters ith node, leaves it or is not incident with it.

The balance scheme in Figure 6 is composed of 11 nodes and 24 streams, nine of which are unmeasured (streams 1-5 are required and streams 6-9 are nonrequired), and 15 streams are measured (10-14 required and 15-24 nonrequired). The unmeasured streams are separately (required and nonrequired) ordered in the sense of increasing measurability. It means, for

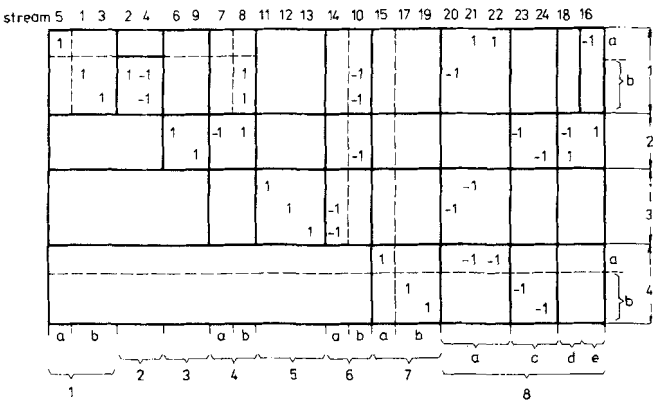

Figure 8. Mathematical model after elimination.

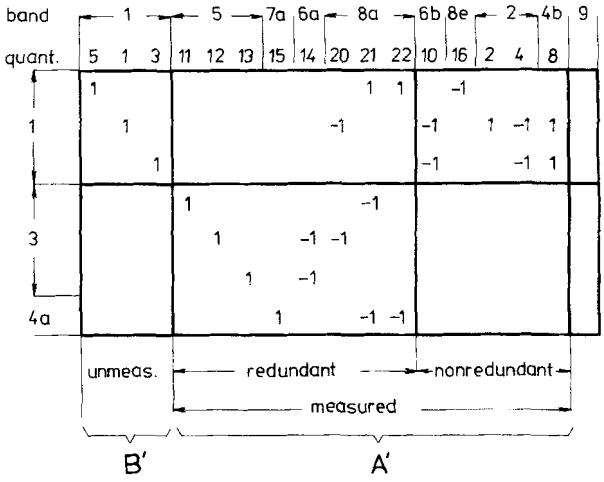

Figure 9. Reduced mathematical model.

example, that stream 2 is more easily measurable than stream 1, and so on.

The set of mass balance equations is of the form (Eq. 1) where $c = 0$; hence, the elimination concerns macromatrix (B, A) only. The macromatrix (B, A) is shown in Figure 7.

The elimination follows the rules according to the Solution of the Problem Section. We successively use pivots in columns 1, 3 and 5, and then in columns 6 and 9. For elimination in the matrix of measured streams, we use, for example, pivots in columns 11, 12 and 13, and then in 15, 17 and 19 (this choice is not unique). After a rearrangement of rows and columns, we obtain the matrix in Figure 8, which corresponds to Figure 4. We assume a diagonal covariance matrix of measurement errors. Then, the equations corresponding to horizontal bands 2 and 4b can be deleted as well as columns representing quantities 6, 7, 9, 17, 19, 23, 24 and 18. Unmeasured quantities 2 and 4 (required) and 8 (nonrequired) have to be measured (we put these columns at the end of matrix A'. Their values are nonredundant and they will not be reconciled. The matrices B' and A' obtained after deletion are shown in Figure 9.

Discussion and Conclusions

The described procedure enables one to realize a complete classification of the quantities and equations occurring in the problem followed by possible optimization of the measurement design. It is based on elimination operations with equations; it can thus be regarded as equation-oriented. It complements other methods based on a graph-theoretical approach developed mostly for balance models (see, for example, algorithms applicable to bilinear constraints previously developed by Kretsovalis and Mah, 1988).

Not discussed is the numeric aspect of the elimination procedure, relevant particularly to ill-conditioned systems (for example, the distinction between a dependent and "almost independent" equation).

We have confined ourselves to mathematical models of the form (Eq. 1). In fact, such systems of equations occur eventually in the identification of nonlinear models that have been linearized.

Briefly discussed are the merits of using the reduced system of equations in a complex measured data processing. A char-

acteristic feature is the decomposition of the problem solution into two steps: a minimum number of redundant measurements are reconciled, and only then, the minimum number of unmeasured parameters is estimated. The main advantage of this data processing is the reduction of the dimension of the problem (reduction of the system of equations and of the dimension of matrices subject to inversion).

The advantages of decomposition are not new and are widely recognized (Crowe et al., 1983). Basically, the decomposition as suggested is algebraically equivalent to that by Crowe et al. (1983) using a matrix projection, which is at present widely used in plant data processing. The presented approach, however, is more detailed (introduction of required and nonrequired quantities, elimination of constraints that are not relevant to the estimation of required quantities, and so on). In comparison with previous methods, the method used in this work (which is based on the well known principle of Gauss-Jordan elimination) appears also more transparent.

Notation

A = matrix of constants in Eq. 1
B = matrix of constants in Eq. 1
c = vector of constants in Eq. 1
I = number of measured quantities
J = number of unmeasured quantities
K = number of Eq. 1
P = set of quantities
P_1 = set of measured quantities
P_2 = set of unmeasured quantities
P_3 = set of required quantities
P_4 = set of nonrequired quantities
$\mathbb{R}$ = set of real numbers
$\mathbb{R}^K$ = $\mathbb{R} \times \ldots \times \mathbb{R}$ (K – times)
x = vector of measured quantities
y = vector of unmeasured quantities

Superscript

T = transposition of a matrix or a vector

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Appendix A: Observability and Redundancy

For the notions and theorems of linear algebra, see, for example, the textbook by MacLane and Birkhoff (1968, Chaps. VII and VIII). In Eq. 1, let V be the $(J + I)$—dimensional vector space of variables (regarded as column vectors):

$$z = \begin{pmatrix} y \\ x \end{pmatrix}$$

where

$$y = (y_1, \ldots y_J)^T \text{ and } x = (x_1, \ldots, x_I)^T \tag{A1}$$

thus, $V = V_y \times V_x$ where V_y (J-dimensional) is space of variables y, V_x (I-dimensional) that of variables x. Let C be the matrix:

$$C = (B,A)$$

$$\text{further let } D = (C,c) \tag{A2}$$

be the extended matrix of the linear system (Eq. 1) of K equations, thus, $c = (c_1, \ldots, c_K)^T \in \mathbb{R}^K$ and C is the matrix of a linear mapping $V \to \mathbb{R}^K$. We can write:

$$C = \begin{pmatrix} \gamma_1 \\ \vdots \\ \gamma_K \end{pmatrix} \tag{A3}$$

where γ_k ($k = 1, \ldots, K$) is the kth row vector of matrix C, thus a linear form $V \to \mathbb{R}$, say $\gamma_k \in V^*$ where V^* is the dual (vector) space to V. Let $e_k \in V$ be the *column* (unit) vector of coordinates δ_{nk} ($\delta_{nk} = 0$ for $n \neq k$, $\delta_{nn} = 1$), then it becomes $(e_1, \ldots, e_{J+I})$ is the canonical basis of V. Let $(\delta_1, \ldots, \delta_{J+I})$ be the canonical dual basis (of V^*) where δ_l is the *row* vector of coordinates δ_{ln}; we thus have:

$$\delta_l \cdot e_k = \delta_{lk}. \tag{A4}$$

If $z_0 \in V$ we introduce the *orthogonal* $z_0^\perp$ as the *vector subspace* of V^* of linear forms ξ such that:

$$\xi \cdot z_0 = 0. \tag{A5}$$

Similarly, if $\xi_0 \in V^*$, then $\xi_0^\perp$ is the vector subspace of V of vectors z such that:

$$\xi_0 \cdot z = 0. \tag{A6}$$

The null space (kernel) of a matrix M is denoted as Ker M; it is thus orthogonal to all row vectors of M.

Now the linear forms $\gamma_1, \ldots, \gamma_K$ generate (by linear combinations) a vector subspace (say) $\tilde{W} \subset V^*$ (where $\tilde{W}$ is a space of row vectors). We have (dimension):

$$\dim \tilde{W} = \tilde{K} \leq K. \tag{A7}$$

If $\tilde{K} = K$, then Eq. 1 is linearly independent and offers some solution to z. If $\tilde{K} < K$ but $\tilde{K} = \text{rank } \boldsymbol{D}$ (Eq. A2), the equations are linearly-dependent, but they admit again some solution to z. If $\tilde{K} < \text{rank } \boldsymbol{D}$ the system (Eq. 1) is inconsistent; this case can be detected (see the main text) and will not be considered. So let $\tilde{K} = \text{rank } \boldsymbol{D}$.

Observe that the space $\tilde{W}$ is generated as well by any other $\tilde{K}$ linearly-independent linear forms obtained on applying the multiplication of $\boldsymbol{C}$ by a regular $K \times K$ matrix $\boldsymbol{R}$ (discarding possibly some $K - \tilde{K}$ zero rows), thus, by a Gauss-Jordan elimination procedure in particular (see the main text). Then, also $\boldsymbol{RD}$ is the extended matrix of a linear system equivalent to Eq. 1. Let us now consider the vector subspace of $\tilde{W}$:

$$\tilde{W}' = \tilde{W} \cap \mathbf{e}_1^{\perp} \cap \ldots \cap \mathbf{e}_J^{\perp} \tag{A8}$$

(intersection of vector spaces). It is the space of row vectors $\alpha \in \tilde{W}$ such that $\alpha \cdot \boldsymbol{e}_j = 0$ for $j = 1, \ldots, J$; we have dim $\tilde{W}' = \tilde{K}' \leq \tilde{K}$, possibly $\tilde{K}' = 0$. Let $H = \text{rank } \boldsymbol{B}$, thus, $H \leq \tilde{K}$; we have:

$$\tilde{K} = H + \tilde{K}'. \tag{A9}$$

Indeed, a basis of $\tilde{K}'$ linearly-independent forms (vectors of $\tilde{W}' \subset \tilde{W}$) can be completed to a basis of $\tilde{W}$ by certain $\tilde{K} - \tilde{K}'$ linearly-independent forms $\beta_h \notin \tilde{W}'$. In the corresponding submatrix of $\tilde{K} - \tilde{K}'$ rows and the first J columns, the rows must be linearly-independent (otherwise, a linear combination of the β_h would eliminate all columns $1, \ldots, J$, thus giving a linear form from $\tilde{W}'$); on the other hand, the rows of the submatrix belong to the space generated by the rows of $\boldsymbol{B}$, thus, $H = \tilde{K} - \tilde{K}'$. The reader may imagine a Gauss elimination transforming $\boldsymbol{C}$ to some $\boldsymbol{RC} = \boldsymbol{C}' = (\boldsymbol{B}', \boldsymbol{A}')$ where $\boldsymbol{B}' = \boldsymbol{RB}$ has the first H rows linearly-independent and the other zero; the remaining $\tilde{K} - H$ linearly-independent rows (zero in columns $1, \ldots, J$) form a basis of $\tilde{W}'$. Schematically,

$$\boldsymbol{RD} = (\boldsymbol{C}', \boldsymbol{c}') = \begin{array}{c} \begin{matrix} \boldsymbol{C}' & & \\ \boldsymbol{B}' & \boldsymbol{A}' & \boldsymbol{c}' \end{matrix} \\ \left(\begin{array}{c|c||c} \boldsymbol{B}_1' & \boldsymbol{A}_1' & \boldsymbol{c}_1' \\ \hline \boldsymbol{0} & \boldsymbol{A}_2' & \boldsymbol{c}_2' \\ & \boldsymbol{0} & \end{array}\right) \begin{matrix} H \\ \tilde{K}' \end{matrix} \end{array} \quad \tilde{K}, \tag{A10}$$

here, rank $\boldsymbol{B}_1' = H$.

It can happen that in addition, $\tilde{W}' \subset \boldsymbol{e}_l^{\perp}$ for some $l > J$. Let L be the set of all such l, thus,

$$\tilde{W}' \subset \boldsymbol{e}_l^{\perp} \text{ for } l \in L \text{ but } \tilde{W}' \not\subset \mathbf{e}_l^{\perp} \text{ for } l > J,\ l \notin L. \tag{A11}$$

The variables $z_l = x_{l-J}$ for $l > J$ are called *nonredundant* if $l \in L$ and *redundant* if $l \notin L$. Clearly, the set of $l \notin L$ is empty if $\tilde{K}' = 0$. In the transformed matrix $\boldsymbol{C}' = \boldsymbol{RC}$ (Eq. A10), if $l \in L$, then all of the lth elements in the last $\tilde{K}' = \tilde{K} - H$ nonzero rows (basis of $\tilde{W}'$) equal zero because $\alpha \cdot \boldsymbol{e}_l = 0$ for any $\alpha \in \tilde{W}'$. If $l' > J$ but $l' \notin L$, then $\alpha \cdot \boldsymbol{e}_{l'} \neq 0$ for some $\alpha \in \tilde{W}'$, thus in particular for some basis (row) vector of $\tilde{W}'$.

Let $\tilde{K}' > 0$. Observe that the linear system with the extended matrix (Eq. A10) is equivalent to the system (Eq. 1). Hence, the system admits a solution in $\boldsymbol{y}$ if and only if $\boldsymbol{A}_2'\boldsymbol{x} + \boldsymbol{c}_2' = \boldsymbol{0}$. This leads to a method of reconciliation as suggested in Madron (1991). If $\boldsymbol{x}^+$ is the vector of actually measured values, the adjusted (reconciled) vector $\hat{\boldsymbol{x}} = \boldsymbol{x}^+ + \boldsymbol{v}$ must satisfy $\boldsymbol{A}_2'\hat{\boldsymbol{x}} + \boldsymbol{c}_2' = \boldsymbol{0}$, thus, $\boldsymbol{A}_2'\boldsymbol{v} + \boldsymbol{b}_2' = \boldsymbol{0}$ where $\boldsymbol{b}_2' = \boldsymbol{A}_2'\boldsymbol{x}^+ + \boldsymbol{c}_2'$. The vector of adjustments $\boldsymbol{v}$ satisfying a generalized least squares criterion is computed according to:

$$\boldsymbol{v} = -\boldsymbol{F}\boldsymbol{A}_2'^{T}(\boldsymbol{A}_2'\boldsymbol{F}\boldsymbol{A}_2'^{T})^{-1}\boldsymbol{b}_2' \tag{A12}$$

where $\boldsymbol{F}$ is $(I \times I)$ covariance matrix of measured values (assumed positive definite). It can be shown formally that the result is independent of the way of transformation (matrix $\boldsymbol{R}$). It is also easy to show that if $\boldsymbol{F}$ is *diagonal*, the components v_l of $\boldsymbol{v}$ for $l \in L$ (nonredundant) equal zero, thus the nonredundant values are nonadjustable. (On the other hand, one can give examples of adjustable nonredundant quantities in the case of a nondiagonal matrix $\boldsymbol{F}$.)

Let us further suppose that the equation $\boldsymbol{A}_2'\boldsymbol{x} + \boldsymbol{c}_2' = \boldsymbol{0}$ is satisfied with some $\boldsymbol{x}$ (for example, $\boldsymbol{x} = \hat{\boldsymbol{x}}$ as above); such value of $\boldsymbol{x}$ can be *compatible* with Eq. 1. Then, any solution $\boldsymbol{y}$ is obtained from $\boldsymbol{B}_1'\boldsymbol{y} + \boldsymbol{b} = \boldsymbol{0}$ where $\boldsymbol{b} = \boldsymbol{A}_1'\boldsymbol{x} + \boldsymbol{c}_1'$ (Eq. A10). If $\boldsymbol{y}'$ is another solution, then $\boldsymbol{y}' - \boldsymbol{y} = \boldsymbol{u}$ where $\boldsymbol{B}_1'\boldsymbol{u} = \boldsymbol{0}$, thus also $\boldsymbol{B}'\boldsymbol{u} = \boldsymbol{0}$ and $\boldsymbol{R}$ being regular, $\boldsymbol{Bu} = \boldsymbol{0}$; hence, $\boldsymbol{u} \in \text{Ker } \boldsymbol{B}$. Let us designate $U = \text{Ker } \boldsymbol{B} = \text{Ker } \boldsymbol{B}' = \text{Ker } \boldsymbol{B}_1'$. Let further $(\delta_{y1}, \ldots, \delta_{yJ})$ be the canonical basis of V_y^* (dual to V_y), thus, δ_{yj} $(j = 1, \ldots, J)$ is the row vector of coordinates δ_{jn} $(n = 1, \ldots, J)$. It can happen that $U \subset \delta_{yj}^{\perp}$ for some j; let N be the set of all such j, thus,

$$U \subset \delta_{yj}^{\perp} \text{ for } j \in N \text{ but } U \not\subset \delta_{yj}^{\perp} \text{ if } j \notin N. \tag{A13}$$

Clearly, if $j \in N$, then the jth component $u_j = \delta_{yj} \cdot \boldsymbol{u} = 0$ for any $\boldsymbol{u} \in U$, hence, $y_j = y_j'$ for any two solutions $\boldsymbol{y}$ and $\boldsymbol{y}'$: the variable y_j is *uniquely determined* by the linear system (Eq. 1), if $\boldsymbol{x}$ is (compatibly) given. If $j' \notin N$, then there is some $\boldsymbol{u} \in U$ such that $u_j \neq 0$, thus, some two solutions $\boldsymbol{y}$ and $\boldsymbol{y}'$ such that $y_j' \neq y_j$; the variable y_j' is *not* uniquely determined. The variables y_j for $j \in N$ are called *observable* and those for $j \notin N$ *unobservable*. In particular, if $J = H$ (regular square $\boldsymbol{B}_1'$), then all y_j are observable.

We have $j \in N$, if and only if the subspace of V_y^* generated by the rows of $\boldsymbol{B}$ (thus of $\boldsymbol{B}_1'$), say $\tilde{B}$ contains δ_{yj}; indeed, $\boldsymbol{Bu} = \boldsymbol{0}$ means $\beta \cdot \boldsymbol{u} = 0$ for any $\beta \in \tilde{B}$, and conversely $\tilde{B}$ is also determined as orthogonal to all vectors of $U = \text{Ker } \boldsymbol{B}$. We thus have the criterion:

$$j \in N \text{ if } \delta_{yj} \in \tilde{B},\ j \notin N \text{ if } \delta_{yj} \notin \tilde{B}. \tag{A14}$$

The criterion can be applied to a matrix $\boldsymbol{B}_1'$ obtained by a Gauss-Jordan elimination procedure (see the main text); if a row of $\boldsymbol{B}_1'$ is δ_{yj} we have $j \in N$ and if no linear combination of the rows yields δ_{yj} then $j \notin N$.

Further, let some variable $x_i = z_{J+i}$ be redundant, thus $J + i \notin L$ (Eq. A11); hence, in some row of $(\boldsymbol{0}, \boldsymbol{A}_2')$ (for some $\alpha \in \tilde{W}'$) we have nonzero element in the $(J + i)$th column. If the variable

x_i is regarded as unmeasured, it can thus be uniquely calculated from the other measured values (it is observable); this is the intuitive interpretation of redundancy.

The spaces $\tilde{W}$, $\tilde{W}'$, U and $\tilde{B}$ and the sets L and N are, according to Eqs. A8, A11, A13 and A14, uniquely determined by the linear system (Eq. 1) and invariant with respect to its equivalent transformations. The system (Eq. 1), as written, corresponds to the partition of the set P of variables (quantities) into subsets P_2 (unmeasured) and P_1 (measured), see the main text. The variables can further be subdivided according to other criteria. If P_3 is the subset of required quantities and P_4 that of nonrequired ones, we have $P_2=(P_2\cap P_3)\cup(P_2\cap P_4)$ and $P_1=(P_1\cap P_3)\cup(P_1\cap P_4)$ as they correspond to the arrangement of our matrix D according to Figure 2; thus, to the corresponding indexation of variables $z_l=y_l$ for $l=1,\ldots,J$ and $z_l=x_{l-J}$ for $l=J+1,\ldots,J+I$. Then, if the subsets $P_1\ldots$ are identified with the subsets of indices, the subsets $N\cap P_3$ ($\subset P_2$ as $N\subset P_2$) and $L\cap P_3$ ($\subset P_1$ as $L\subset P_1$), as well as $L\cap P_4$ ($\subset P_1$) are again uniquely determined. By a Gauss-Jordan elimination procedure, we obtain matrix (C',c') (Eq. A10) according to Figure 4 (where we now assume $\tilde{K}=\text{rank } D$). According to the procedure, the subsets of columns 1 and 2 (thus, $P_2\cap P_3$), 3 and 4 (thus $\subset P_2\cap P_4$), 5 and 6 (thus $P_1\cap P_3$), 7 and 8 (thus $P_1\cap P_4$) are rearranged (each separately), which corresponds to a rearrangement of variables. Then, the columns 1*a* represent $z_j=y_j$ for $j\in N\cap P_3$, and the columns 1*b* and 2 correspond to $j\in P_2\cap P_3$ but $j\notin N$; the subset $N\cap P_4$ ($\subset P_2\cap P_4$) is not specified (it would be represented by certain columns of group 3) because the values are not required. Further, the columns 6*b* represent $z_l=x_{l-J}$ for $l\in L\cap P_3$ and the columns 8*de* correspond to $l\in L\cap P_4$. By an analogous consideration as above [see the introduction of $\tilde{W}'$ (Eq. A8)], it can be shown that also the subspace of $\tilde{B}$ generated by row 2 restricted to columns 1-4, and the subspace of $\tilde{W}'$ generated by row 4 are uniquely determined.

Further finer subdivision in Figure 4 (for example, into 1*b* and 2, 5 and 6*a*, and so on) is no more unique algebraically; it depends on the elimination procedure. The procedure, however, is "optimized" in a manner explained in the main text. See also Appendix C.

Appendix B: Matrix Decomposition

The submatrix $Z_{4,8abc}$ in Figure 4 is arranged using an algorithm elaborated by the authors. The rearrangement of the matrix $Z_{4,8}$ proceeds as follows.

After the matrix rearrangements according to points 1 to 6 of the main text (in the columns of the groups 1-6), one obtains submatrices in Figure 4. But so far, the rearrangements in columns 7, 8 and 9 have led to the format shown in Figure A1 where b' stands for bc. The desired rearrangement of submatrix $Z_{4,8ab'}$ according to point 7 is carried out in two steps.

1. Consider that the rearrangement differentiate zero and nonzero elements only. Let us thus imagine a $K\times L$ matrix A where $A_{kl}=0$ or 1; $A_{kl}=1$ stands for $A_{kl}\neq 0$. The indices $k\in K$ and $l\in L$ are certain addresses in the lists of rows (equations) K and columns (variables) L arbitrarily ordered: kl thus uniquely determines the corresponding matrix element. From the sets K and L, we first separate the groups K^0 of zero rows and L^0 of zero columns. The remaining matrix $\overline{A}$ is of the type

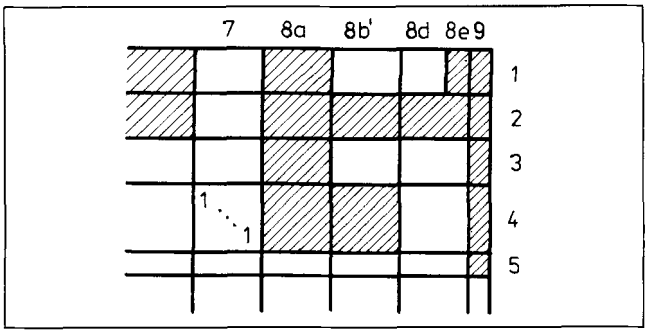

Figure A1. Decomposition of a matrix.

(say) $\overline{K}\times\overline{L}$. It can be said that there exists (within the order) just one disjoint decomposition $K=\overline{K}_1\cup\ldots\cup\overline{K}_r$, $L=\overline{L}_1\cup\ldots\cup\overline{L}_r$ such that the submatrices (blocks)

$$\mathbf{A}^{(ij)}=(A_{kl})_{\substack{k\in\overline{K}_i\\ l\in\overline{L}_j}}\quad(i,j=1,\ldots,r)\tag{B1}$$

are zero for $i\neq j$ and nonzero "connected" for $i=j$. The "connectedness" of a matrix $A^{(ii)}$ means that no further rearrangement can result in a finer subdivision into blocks of the type shown in Figure A2.

A precise algebraic formulation and proof are possible, but will not be given here. Let us only indicate an algorithm leading to the desired decomposition.

(0) Find (k_0,l_0) such that $A_{k_0l_0}=1$ (thus, $\neq 0$ in matrix $Z_{4,8ab'}$).

(1) For column l_0, find all k such that $A_{kl_0}=1$: get $K^{(1)}\subset\overline{K}$.

(2) Go successfully through rows $k\in K^{(1)}$ and write for each k all l such that $A_{kl}=1$; in the total get set $L^{(1)}\subset\overline{L}$.

(3) Go successively through columns $l\in L^{(1)}$ and write for each l all k such that $A_{kl}=1$: in the total get set $K^{(2)}\supset K^{(1)}$ and so on.

After a finite number of steps, we will have $K^{(m+1)}=K^{(m)}$ and $L^{(m+1)}=L^m$, and we can set $\overline{K}_1=K^{(m)}$, $\overline{L}_1=L^{(m)}$. And then, we arrive at the first block $\mathbf{A}^{(11)}$: $\overline{K}_1\times\overline{L}_1$ of the sought decomposition. Further, one finds (if they exist) $k_1\notin\overline{K}_1$, $l_1\notin\overline{L}_1$ such that $A_{k_1l_1}=1$ and so on, and finally get the whole decomposition. The algorithm is of the order α^3 at most, where $\alpha=\max'$ (number of rows and number of columns).

2. By this arrangement of matrix $Z_{4,8ab'}$, we have reordered

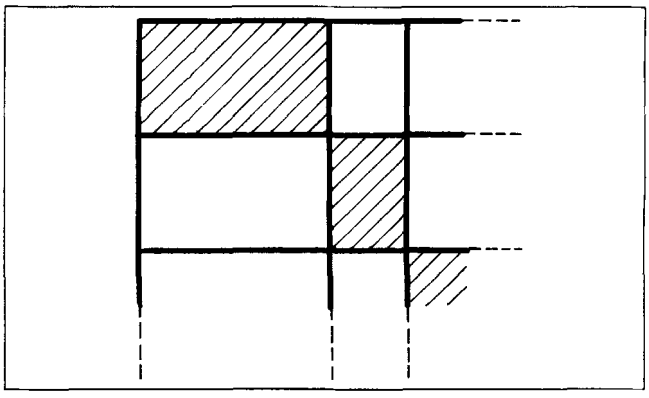

Figure A2. Decomposition of a matrix.

the columns $8ab'$ (the set $\overline{L}$; the columns of subset L^0 can be left in their initial places). Now from the subsets $\overline{L}_i$ $(i=1,\ldots,r)$ we select those which are whole in the initial $8a$ and those which are whole in $8b'$, and place them on the respective groups (vertical bands); there remain certain columns L' to which our decomposition cannot be applied (see the rule in point 7) of the main text concerning the matrix rearrangements). So, the set L' is regrouped into columns L'_a lying in $8a$ and L'_b lying in $8b'$. To the set L' corresponds uniquely, according to the decomposition in step 1, a certain group of rows K' nonzero in the submatrix $K' \times L'$. With an appropriate ordering, $\overline{L}_1 \cup \ldots \cup \overline{L}_{r_\alpha}$ lies in $8a$, nonzero are just $\overline{K}_1 \times \overline{L}_1, \ldots, K_{r_\alpha} \times \overline{L}_{r_\alpha}$, and further $K' \times L'$ is nonzero, while the remaining rows (being neither in $\overline{K}_1 \cup \ldots \cup \overline{K}_{r_\alpha}$ nor in K') have zeros in columns $\overline{L}_1 \cup \ldots \cup \overline{L}_{r_\alpha} \cup L'$ thus in columns $8a$ and L'_b. The columns L'_b thus will form group $8b$ and the remaining ones (when they exist) form group $8c$, while the given partition of rows generates groups $4a$ and $4b$ as shown in Figure 4. Having reordered the rows of band 4, we finally can reorder the columns of group 7 accordingly to have again diagonal matrix $Z_{4,7}$. Recall that the band $4b$ can also be empty.

Appendix C: Choice of Additional Measurements

Modifying the notation in Appendix A, let $y_1, \ldots, y_A$ be the required unmeasured quantities and $y'_1, \ldots, y'_B$ be the nonrequired unmeasured ones; thus, $A+B=J$. Separate orders increase measurability. Let us follow the elimination procedure as suggested in the main text with Figure 4.

Elimination begins with columns 1 and 2 corresponding to y_j, $J=1,\ldots,A$. Reordering the columns will yield the order $k_1,\ldots,k_A$ which is permutation of numbers $1,\ldots,A$. We have $k_1=1$ (otherwise, $j=1$ would be zero column, a case not considered here). Now k_2 is the smallest number $k_2>1$ such that the elimination can go on. The columns between k_1 and k_2 (if present) have just one nonzero element, this in the same row as column $k_1=1$ after the first elimination step. This means that the submatrix of columns $1,\ldots,k_2-1$ is of rank 1 (which is independent of the elimination procedure). The columns between k_1 and k_2 are placed at the end and are not used for elimination. Generally, if there are such columns between some k_r and k_{r+1}, then the submatrix of columns $1,\ldots,k_r,\ldots,k_{r+1}-1$ is of the rank r, the columns being linear combinations of columns $k_1,\ldots,k_r$ (which are linearly-independent). In other words, we always choose the smallest number k_{r+1} which can follow after k_r, with $k_1 < k_2 < \ldots k_r$, and this choice is *independent* of the choice of admissible pivots and of the order of rows. The number of columns 1, say C, is determined uniquely by the linear system; it is the rank of the restriction of matrix $\boldsymbol{B}$ to the variables $y_1,\ldots,y_A$. We thus always obtain just C columns, generally $k'_1,\ldots,k'_C$ by an arbitrary elimination procedure. If S is the set of indices $k_1,\ldots,k_C$ and S' that of $k'_1,\ldots,k'_C$, then in $S \cap S'$ any $k'_{r'}$ equals just some k_r, while if $k'_{s'} \notin S \cap S'$, we have $k'_{s'} > k_s$ whatever be $k_s \in S$ according to the construction of S. Hence,

$$\sum_{l=1}^{C} k_l \leq \sum_{l=1}^{C} k'_l \qquad \text{(C1)}$$

where the equality holds only if $S=S'$.

If it happens that all nonrequired unmeasured variables are observable (or simply absent), the subset of columns 4 is void and the variables 3 need not be measured; this case is detected by the procedure and the only additional measurements will concern the variables $1b$ and 2. The choice of the variables y_j where $j=k_1,\ldots,k_C$ as those which need *not* be measured is then optimal in the sense of minimum sum of orders (Eq. C1). The latter criterion is satisfied in any case. But generally, one has to measure also certain values corresponding to $4b$. It can be shown that the sum of orders in subset 3 is again minimum, but generally also some variables $4a$ need *not* be measured. The number of columns $4b$ is not algebraically invariant and is thus difficult to compare two different choices of additionally measured nonrequired quantities; another choice could perhaps reduce the number of *theoretically* necessary additional measurements (as can be shown on examples), but such possibility remains generally unknown. Hence, from the practical point of view, the suggested method of elimination appears to be the best.

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