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NUCLEAR-DATA EVALUATION BASED ON DIRECT AND INDIRECT MEASUREMENTS WITH GENERAL CORRELATIONS

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Abstract: Optimum procedures for the statistical improvement, or updating, of an existing nuclear-data evaluation are reviewed and redeveloped from first principles, consistently employing a minimum-variance viewpoint. A set of equations is derived which provides improved values of the data and their covariances, taking into account information from supplementary measurements and allowing for general correlations among all measurements. The minimum-variance solutions thus obtained, which we call the method of "partitioned least squares," are found to be equivalent to a method suggested by Yu. V. Linnik and applied by a number of authors to the analysis of fission-reactor integral experiments; however, up to now, the partitioned-least-squares formulae have not found widespread use in the field of basic data evaluation. This approach is shown to give the same results as the more commonly applied Normal equations, but with reduced matrix inversion requirements. Examples are provided to indicate potential areas of application.

(data evaluation, updating, adjustment, minimum variance, Gauss-Markov theorem, normal equations, least squares, correlation, uncertainty analysis)

Introduction

Many problems in the general field of data evaluation reduce to the need to update an existing data set, taking into account a relatively small number of supplementary measurements, performed directly on the data or on certain functions of the data. A very useful tool for accommodating the new information is the method of correlated linear least squares.

The equations usually solved in applying the method of correlated linear least squares, the "Normal" equations, can be derived from a wide variety of starting points, but many authors, ranging from C. F. Gauss[1] to R. W. Peelle,[2] have preferred to view these equations as a method for minimizing the uncertainty in physical data, given a set of measurements and their uncertainties. In the language of statistics, correlated linear least squares (CLLS) is viewed as a method for constructing minimum-variance linear unbiased estimators of the true data values. In a result known as the Gauss-Markov theorem, the Normal equations have been shown[1,3,4] to provide minimum-variance estimates, not only of the data, but also of every linear function of the data, an important consideration in data applications. The proof of the Gauss-Markov theorem does not require any assumptions regarding the shape of the probability distributions of the measurements, except that the distributions have finite second moments. The power and general applicability of the CLLS method probably account for its wide use.

The particular formulation of the CLLS method that is most appropriate for the task at hand, namely the updating of an existing data set, does not require the full generality of the standard form of the Normal equations, as given for example in Eq. (24) below, because, in the case of updating, the sensitivity matrix **H** relating the measured quantities to the parameters has a special "partitioned" structure. As shown below, it is possible to take advantage of this special structure of the sensitivity matrix to reduce the matrix-inversion requirements relative to solving the Normal equations, while still retaining the minimum-variance guarantees.

The updating of existing data evaluations also differs from other applications of the CLLS method in that the number of data values in the pre-existing set is often much larger than the number of new measurements. This provides considerable motivation for finding approaches which avoid the inversion of the large, joint covariance matrix of the old and new measurements. An algorithm that accomplishes this reduction in matrix-inversion requirements was given in a textbook by Yu. V. Linnik[5] and was later developed into a method for fission-reactor integral-experiment analysis (or "data adjustment") by A. Gandini and co-workers[6,7] and by J. Marable and co-workers[8-10], who emphasized the need to treat correlations between the class of existing data and the new measurements.

The theoretical justifications offered in Refs. 5-10 are fundamentally "Bayesian"; that is, the measurements are assumed to be sampled from normal distributions, and the adjustment equations are then obtained by appeal to the principle of maximum likelihood. It was noted in Ref. 2, in connection with the development of the Normal equations, that arguments based on assumed normal probability distributions do not seem to offer guarantees that are as strong as those given by the minimum-variance approach, because non-normal probability distributions are frequently encountered.

Essentially all of the work reported in Refs. 6-10 was motivated by programs in fission-reactor design and technology. These same adjustment formulae also appear to have a promising role in the field of critical evaluation of nuclear data, as well as other kinds of data. Because of the potential for future application by a very broad community of users, we have re-examined the subject of updating an existing evaluation, starting from first principles and consistently employing the viewpoint of minimum-variance estimation.

Statement of the Problem

We suppose that there exists a data set $[a_j, j=1,k]$ corresponding to the measurement (or evaluation) of k different physical parameters (for example, the ground-state masses of k different nuclei, or a nuclear-reaction cross

section at k different neutron energies) having true values x_j. In each case, the measurement is assumed to differ from the true value by a random error e_j, that is, $a_j = x_j + e_j$. The errors e_j are assumed to have zero mean, so that $E(a_j) = x_j$. We employ the symbol E( ) to indicate the expectation value of a scalar, vector or matrix, obtained by averaging each element over the probability distribution of the errors. We consider a_j, x_j and e_j to be elements of the column vectors **a**, **x** and **e**, respectively. In vector notation, then,

$$E(\mathbf{a}) = \mathbf{x}, \tag{1}$$

It is also assumed that the errors e_j have finite second moments, given by the covariance or "dispersion" matrix D(**a**),

$$D(\mathbf{a}) = \mathrm{cov}(\mathbf{a},\mathbf{a}) = E(\mathbf{e}\,\mathbf{e}^T),$$

where the $(^T)$ symbol indicates the matrix transpose. Since **e** is a column vector, $\mathbf{e}^T$ is a row vector having the same elements, and $[\mathbf{e}\,\mathbf{e}^T]$ is a square matrix of dimension k.

The vector **a** and the covariance matrix D(**a**) introduced above describe the status of one's knowledge of the parameters prior to the performance of a set of new measurements. The expected value of each of these new observations $[b_i, i=1,m]$ is some function of the parameters **x**. All such functions are assumed here to be either linear or "linearized." That is, we assume that nonlinearities are either absent or small enough to be neglected in calculating variances. We also assume that, if the problem is nonlinear, a suitable change of variables has been performed, absorbing the reference values for the linear expansion into the definitions of both the parameters and the measurement vectors **a** and **b**.

As before, there is a random error f_i associated with each measurement b_i, causing the measurement to differ from the expected value,

$$b_i = R_{i1}\,x_1 + R_{i2}\,x_2 + \ldots + R_{ik}\,x_k + f_i,$$

where R_{ij} is the ij-th element of the m x k sensitivity, or derivative, matrix **R**. The errors are assumed to have zero mean values, so that

$$E(\mathbf{b}) = \mathbf{R}\,\mathbf{x}. \tag{2}$$

As with **a**, the second moments of **b** are given by $D(\mathbf{b}) = E(\mathbf{f}\,\mathbf{f}^T)$. "Cross-type" covariances, indicating correlations between the old and new measurements, are defined analogously; $\mathrm{cov}(\mathbf{a},\mathbf{b}) = E(\mathbf{e}\,\mathbf{f}^T)$ and $\mathrm{cov}(\mathbf{b},\mathbf{a}) = E(\mathbf{f}\,\mathbf{e}^T)$, so that

$$\mathrm{cov}(\mathbf{b},\mathbf{a}) = [\mathrm{cov}(\mathbf{a},\mathbf{b})]^T.$$

It is important to emphasize that the covariance matrices D(**a**), D(**b**) and cov(**a**,**b**) describe properties of the experimental (or evaluation) errors **e** and **f**, which, in turn, depend only on the experiments employed. These uncertainties and correlations are not related in any way to the fact that E(**a**) and E(**b**) are both functions of the same parameter set **x**. The main point of the CLLS method is that the logical connection between the two sets of expectation values, Eqs. (1) and (2), is additional information that can be used to reduce the uncertainty in one's knowledge of the parameters **x**.

Examples of Possible Applications

Before proceeding to a discussion of how this reduced uncertainty can be attained, it is useful to illustrate the idea of measurement correlations by considering some particular examples. Suppose an experimenter measures the energy-dependent neutron cross section for a particular nuclear reaction by counting activation gamma rays, and the same experimenter also measures, with the same method, the reaction rate for this reaction within a large integral assembly irradiated by an external neutron source. The first measurement may be important in evaluating the differential cross sections **a**, while the second one may be proposed as an integral measurement **b** to be used in improving, or adjusting, **a**. Potential sources of error which are common to the two measurements (e. g., uncertainty in the efficiency of the gamma-ray detector) can introduce substantial measurement correlations in such a case. Integral-differential measurement correlations also can arise when cross-section measurers, on the one hand, and integral experimenters, on the other hand, both rely on a common datum, such as a decay half-life, in reducing their data.

It is easy to imagine other situations that have a partitioned character and significant "cross-type" correlations, but do not involve neutronics integral experiments. If the number of parameters is large, it may be very advantageous to analyze these cases, also, with the partitioned form of least squares rather than the standard form. For example, suppose an experimental nuclear physics group measures the energy-dependent neutron cross sections for five individual nuclear reactions, as well as the total cross section (assumed equal, by definition, to the sum of the individual ones) at each of 200 neutron energies. Correlations can clearly exist between any of these 1200 measurements and any other one. An obvious choice for the parameter set **x** is the set of true values of the individual cross sections, so that k = 1000. Application of the standard form of the CLLS method would require the inversion of a matrix of dimension 1200. As shown below, the same results can be obtained by inverting only the covariance matrix of the "discrepancy" vector (the differences **b - R a** between the measured "totals" and the sums of the measured "partials"), which would be of dimension 200.

Partitioned Formulation of Correlated Linear Least Squares

We assume that, for a given application, the goal is to find best estimates of the true values **x** of the parameters or, more generally, best estimates of certain fixed linear combinations of the **x**. In developing a strategy to accomplish this, it will prove convenient to introduce a new vector **z** with n elements, each defined as a certain linear combination of all observations,

$$\mathbf{z} = \mathbf{S}\,\mathbf{a} + \mathbf{T}\,\mathbf{b}. \tag{3}$$

The true (or expectation) values of the **z** are then given by

$$E(\mathbf{z}) = \mathbf{S}\,E(\mathbf{a}) + \mathbf{T}\,E(\mathbf{b}),$$

or,

$$E(\mathbf{z}) = \mathbf{S}\,\mathbf{x} + \mathbf{T}\,\mathbf{R}\,\mathbf{x}\ .$$

We can characterize the above-stated goal as that of finding a best estimate of E(**z**), given **S** and **T**. In other words, **S** and **T** together define a unique "application." It will turn out that the constant matrices **S** and **T** affect the minimum-variance solution only through their effect on

the magnitude of the auxiliary quantity $\mathbf{z}$, so they need not be specified in advance. The important situation where one wishes to adjust the existing differential data set is included as the special case [$n = k$, $\mathbf{S} = \mathbf{I}$ (the identity matrix), and $\mathbf{T} = 0$], that is, $\mathbf{z} = \mathbf{a}$. The reverse situation, where one wants to use the differential data to improve the integral data, $\mathbf{z} = \mathbf{b}$, is a similar special case.

We now introduce $\mathbf{z}'$, to be constructed as a minimum-variance linear unbiased estimator of the quantity $E(\mathbf{z})$ above. Initially, we take $\mathbf{z}'$ to be an arbitrary linear combination of all available measured data

$$\mathbf{z}' = \mathbf{V}\,\mathbf{a} + \mathbf{W}\,\mathbf{b}, \tag{4}$$

the strategy being to find values of the elements of the weight matrices $\mathbf{V}$ and $\mathbf{W}$ that minimize the variances of the individual elements of $\mathbf{z}'$.

Since we require $\mathbf{z}'$ to be unbiased, $E(\mathbf{z}')$ must be equal to $E(\mathbf{z})$. This restricts the choices available for the weights as follows:

$$\mathbf{V}\,E(\mathbf{a}) + \mathbf{W}\,E(\mathbf{b}) = \mathbf{S}\,E(\mathbf{a}) + \mathbf{T}\,E(\mathbf{b}),$$

and from Eqs. (1) and (2),

$$\mathbf{V}\,\mathbf{x} + \mathbf{W}\,\mathbf{R}\,\mathbf{x} = \mathbf{S}\,\mathbf{x} + \mathbf{T}\,\mathbf{R}\,\mathbf{x}.$$

The true values $\mathbf{x}$ of the parameters are unknown; thus, to guarantee an unbiased solution $\mathbf{V}$ and $\mathbf{W}$ must be chosen to satisfy the relation

$$\mathbf{V} = \mathbf{S} + \mathbf{T}\,\mathbf{R} - \mathbf{W}\,\mathbf{R}.$$

This condition on $\mathbf{V}$ and $\mathbf{W}$ implies that Eq. (4) can be re-written as

$$\mathbf{z}' = \mathbf{S}\,\mathbf{a} + \mathbf{T}\,\mathbf{R}\,\mathbf{a} - \mathbf{W}\,\mathbf{R}\,\mathbf{a} + \mathbf{W}\,\mathbf{b},$$

or, substituting from Eq. (3),

$$\mathbf{z}' = \mathbf{z} + (\mathbf{W} - \mathbf{T})\,(\mathbf{b} - \mathbf{R}\,\mathbf{a}).$$

We note that the vector $\mathbf{R}\,\mathbf{a}$ contains the values of the newly measured quantities, as calculated with the old evaluation of the parameters. We introduce the notation $\mathbf{p}$ for this "discrepancy" vector

$$\mathbf{p} = \mathbf{b} - \mathbf{R}\,\mathbf{a}, \tag{5}$$

so that

$$\mathbf{z}' = \mathbf{z} + (\mathbf{W} - \mathbf{T})\,\mathbf{p}. \tag{6}$$

From the definition in Eq. (5), the covariance matrix for $\mathbf{p}$ can be written

$$D(\mathbf{p}) = \mathrm{cov}(\mathbf{p},\mathbf{p}) = D(\mathbf{b}) - \mathrm{cov}(\mathbf{b},\mathbf{a})\,\mathbf{R}^T - \mathbf{R}\,\mathrm{cov}(\mathbf{a},\mathbf{b}) + \mathbf{R}\,D(\mathbf{a})\,\mathbf{R}^T.$$

In finding the optimum choice for the elements of the still-arbitrary matrix $\mathbf{W}$, it will prove convenient to introduce a second arbitrary matrix $\mathbf{Q}$, related to $\mathbf{W}$ by

$$\mathbf{W} - \mathbf{T} = \mathbf{Q} - \mathrm{cov}(\mathbf{z},\mathbf{p})\,\mathbf{G}, \tag{7}$$

where

$$\mathbf{G}^{-1} = D(\mathbf{p}). \tag{8}$$

Utilizing Eqs. (6), (7) and (8), we now can write an expression for the uncertainties of the $\mathbf{z}'$ that result from the uncertainties the quantities $\mathbf{z}$ and $\mathbf{p}$ (which, in turn, depend on the measured quantities $\mathbf{a}$ and $\mathbf{b}$).

$$D(\mathbf{z}') = \mathrm{cov}\{[\mathbf{z} + \mathbf{Q}\,\mathbf{p} - \mathrm{cov}(\mathbf{z},\mathbf{p})\,\mathbf{G}\,\mathbf{p}], [\mathbf{z} + \mathbf{Q}\,\mathbf{p} - \mathrm{cov}(\mathbf{z},\mathbf{p})\,\mathbf{G}\,\mathbf{p}]\}$$

$$= D(\mathbf{z}) + D(\mathbf{Q}\,\mathbf{p}) - \mathrm{cov}(\mathbf{z},\mathbf{p})\,\mathbf{G}\,\mathrm{cov}(\mathbf{p},\mathbf{z}). \tag{9}$$

In arriving at this last result, extensive use of Eq. (8) has been made in collapsing the original nine covariance contributions down to just three.

The diagonal elements of $D(\mathbf{Q}\,\mathbf{p})$ in Eq. (9) are variances and cannot be made negative by any choice of $\mathbf{Q}$. However, they can be made equal to zero (by setting all elements of $\mathbf{Q}$ equal to 0). Thus, the minimum-variance estimator $\mathbf{z}'$, the one with the smallest "error bars," is obtained by substituting $\mathbf{Q} = 0$ in Eqs. (6), (7) and (9);

$$\mathbf{z}' = \mathbf{z} - \mathrm{cov}(\mathbf{z},\mathbf{p})\,\mathbf{G}\,\mathbf{p}, \tag{10}$$

$$D(\mathbf{z}') = D(\mathbf{z}) - \mathrm{cov}(\mathbf{z},\mathbf{p})\,\mathbf{G}\,\mathrm{cov}(\mathbf{p},\mathbf{z}) \tag{11}$$

$$= D(\mathbf{z}) - D[\mathrm{cov}(\mathbf{z},\mathbf{p})\,\mathbf{G}\,\mathbf{p}]. \tag{12}$$

The "adjustment" equations, Eqs. (10) and (11), are the desired minimum-variance solution to the partitioned-least-squares problem for the case of measurements with general correlations. We note immediately that (as desired) the largest covariance matrix that needs to be inverted, $D(\mathbf{p})$, is of order of the number of new indirect measurements, and that no restrictions have been placed on measurement correlations. We also note from the form of Eq. (12) that the uncertainties of the z_i' are guaranteed to be less than those of the original z_i.

The adjustment equations can now be specialized to various applications by making particular choices for $\mathbf{S}$ and $\mathbf{T}$. For example, solutions for the parameters themselves are obtained by specifying that the quantity of interest is simply $\mathbf{z}_1 = \mathbf{a}$. Solutions for the parameters are then obtained immediately from Eqs. (10) and (11). Introducing the obvious notation of $\mathbf{a}'$ for the solution in this case,

$$\mathbf{a}' = \mathbf{a} - \mathrm{cov}(\mathbf{a},\mathbf{p})\,\mathbf{G}\,\mathbf{p}, \tag{13}$$

$$D(\mathbf{a}') = D(\mathbf{a}) - \mathrm{cov}(\mathbf{a},\mathbf{p})\,\mathbf{G}\,\mathrm{cov}(\mathbf{p},\mathbf{a}), \tag{14}$$

where, recalling Eq. (5), we have

$$\mathrm{cov}(\mathbf{a},\mathbf{p}) = \mathrm{cov}(\mathbf{a},\mathbf{b}) - D(\mathbf{a})\,\mathbf{R}^T. \tag{15}$$

A second interesting case is the general linear function $\mathbf{z}_2 = \mathbf{S}\,\mathbf{a}$. Again from Eq. (10), and using the fact that $\mathrm{cov}(\mathbf{z}_2,\mathbf{p}) = \mathbf{S}\,\mathrm{cov}(\mathbf{a},\mathbf{p})$,

$$\mathbf{z}_2' = \mathbf{S}\,\mathbf{a} - \mathbf{S}\,\mathrm{cov}(\mathbf{a},\mathbf{p})\,\mathbf{G}\,\mathbf{p} = \mathbf{S}\,[\mathbf{a} - \mathrm{cov}(\mathbf{a},\mathbf{p})\,\mathbf{G}\,\mathbf{p}] = \mathbf{S}\,\mathbf{a}'. \tag{16}$$

This result is the equivalent of the Gauss-Markov theorem for the partitioned case. The practical importance of this is that the minimum-variance estimate of the parameters, $\mathbf{a}'$, can be used to calculate directly the minimum-variance estimate of any linear function of the parameters, without actually repeating the adjustment exercise.

Finally, we consider the special case in which one wishes to produce improved estimates of the indirect measurements, $\mathbf{z}_3 = \mathbf{b}$. Again, we have from Eqs. (10) and (11)

$$\mathbf{b}' = \mathbf{b} - \mathrm{cov}(\mathbf{b},\mathbf{p})\,\mathbf{G}\,\mathbf{p}, \tag{17}$$

$$D(\mathbf{b}') = D(\mathbf{b}) - \mathrm{cov}(\mathbf{b},\mathbf{p})\,\mathbf{G}\,\mathrm{cov}(\mathbf{p},\mathbf{b}), \tag{18}$$

where, again from Eq. (5), we have

$$\mathrm{cov}(\mathbf{b},\mathbf{p}) = D(\mathbf{b}) - \mathrm{cov}(\mathbf{b},\mathbf{a})\,\mathbf{R}^T. \tag{19}$$

It is useful now to place our results in the context of earlier work along similar lines. Interestingly, except for minor notational differences, the minimum-variance solutions that we obtain in Eqs. (13)-(19) are identical to the adjustment equations of Refs. 5-10, which were derived from maximum-likelihood arguments. The fact that these formulae can be derived in a

variety of ways strongly suggests that they are, in fact, just the Normal equations, specialized to the partitioned case. The nested matrix inversions of the standard form of the Normal equations (see below) makes this connection less than obvious, so we present below a direct demonstration that solutions of the adjustment equations are also solutions of the Normal equations.

The connection with the Normal equations is most compactly presented in terms of partitioned matrices for the measurement vector $\mathbf{y}$, the measurement errors $\mathbf{u}$, and the associated covariance matrix.

$$\mathbf{y} = \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix}, \qquad \mathbf{u} = \begin{bmatrix} \mathbf{e} \\ \mathbf{f} \end{bmatrix},$$

$$D(\mathbf{y}) = E(\mathbf{u}\,\mathbf{u}^T) = \begin{bmatrix} D(\mathbf{a}) & \mathrm{cov}(\mathbf{a},\mathbf{b}) \\ \mathrm{cov}(\mathbf{b},\mathbf{a}) & D(\mathbf{b}) \end{bmatrix}$$

Similarly, we introduce the partitioned matrix

$$\mathbf{C} = [-\mathbf{R}_{m,k} \mid \mathbf{I}_{m,m}], \tag{20}$$

where the submatrix dimensions are indicated by subscripts. The discrepancy vector can then be written as

$$\mathbf{p} = \mathbf{b} - \mathbf{R}\,\mathbf{a} = \mathbf{C}\,\mathbf{y}.$$

We also introduce the matrix

$$\mathrm{cov}(\mathbf{y},\mathbf{p}) = \begin{bmatrix} \mathrm{cov}(\mathbf{a},\mathbf{p}) \\ \mathrm{cov}(\mathbf{b},\mathbf{p}) \end{bmatrix}$$

so that the partitioned-least-squares solutions, Eqs. (13) and (17), can be combined.

$$\mathbf{y}' = \begin{bmatrix} \mathbf{a}' \\ \mathbf{b}' \end{bmatrix} = \mathbf{y} - \mathrm{cov}(\mathbf{y},\mathbf{p})\,\mathbf{G}\,\mathbf{p}. \tag{21}$$

Noting that

$$\mathrm{cov}(\mathbf{y},\mathbf{p}) = \mathrm{cov}(\mathbf{y},\mathbf{C}\,\mathbf{y}) = D(\mathbf{y})\,\mathbf{C}^T,$$

we can re-write Eq. (21) as

$$\mathbf{y}' = \mathbf{y} - D(\mathbf{y})\,\mathbf{C}^T\,\mathbf{G}\,\mathbf{p}. \tag{22}$$

We introduce another partitioned matrix $\mathbf{H}$, where

$$\mathbf{H}^T = [\mathbf{I}_{k,k} \mid \mathbf{R}^T_{k,m}]. \tag{23}$$

The matrix $\mathbf{H}$ is the "partitioned sensitivity matrix" mentioned in the Introduction. In terms thus defined, the "observation equations" of the standard CLLS approach become

$$\mathbf{y} = \mathbf{H}\,\mathbf{x} + \mathbf{u}.$$

Given $\mathbf{y}$, $D(\mathbf{y})$ and $\mathbf{H}$, the CLLS method obtains best estimates $\mathbf{d}'$ of the parameters $\mathbf{x}$ as solutions of the Normal equations, for example Eq. (27) of Ref. 2,

$$\mathbf{d}' = [\mathbf{H}^T D^{-1}(\mathbf{y})\,\mathbf{H}]^{-1}\,\mathbf{H}^T D^{-1}(\mathbf{y})\,\mathbf{y}. \tag{24}$$

We now show that the parameter portion $\mathbf{a}'$ of the solutions $\mathbf{y}'$ of Eq. (22) are identical to the solutions $\mathbf{d}'$ of Eq. (24). We multiply both sides of Eq. (22) by $D^{-1}(\mathbf{y})$, giving

$$D^{-1}(\mathbf{y})\,\mathbf{y}' = D^{-1}(\mathbf{y})\,\mathbf{y} - \mathbf{C}^T\,\mathbf{G}\,\mathbf{p}.$$

We then multiply by $\mathbf{H}^T$ and obtain

$$\mathbf{H}^T D^{-1}(\mathbf{y})\,\mathbf{y}' = \mathbf{H}^T D^{-1}(\mathbf{y})\,\mathbf{y} - \mathbf{H}^T\,\mathbf{C}^T\,\mathbf{G}\,\mathbf{p}. \tag{25}$$

Manipulating Eqs. (14) and (17), one can show that

$$\mathbf{b}' = \mathbf{R}\,\mathbf{a}',$$

so that $\mathbf{y}'$ and $\mathbf{a}'$ satisfy the relation

$$\mathbf{y}' = \begin{bmatrix} \mathbf{a}' \\ \mathbf{b}' \end{bmatrix} = \begin{bmatrix} \mathbf{a}' \\ \mathbf{R}\,\mathbf{a}' \end{bmatrix} = \mathbf{H}\,\mathbf{a}'.$$

Another useful intermediate result is that

$$\mathbf{H}^T\,\mathbf{C}^T = \mathbf{R}^T - \mathbf{R}^T = 0.$$

Substituting for $\mathbf{y}'$ and $\mathbf{H}^T\,\mathbf{C}^T$ in Eq. (25), we obtain

$$\mathbf{H}^T D^{-1}(\mathbf{y})\,\mathbf{H}\,\mathbf{a}' = \mathbf{H}^T D^{-1}(\mathbf{y})\,\mathbf{y}.$$

Multiplying through by $[\mathbf{H}^T D^{-1}(\mathbf{y})\,\mathbf{H}]^{-1}$ then gives the desired result. Provided that the sensitivity matrix $\mathbf{H}$ has the required "adjustment" character, Eq. (23), and provided that a solution of the Normal equations exists, then the partitioned least-squares solutions $\mathbf{a}'$ are identical to the solutions $\mathbf{d}'$ of the Normal equations. In addition to computational efficiency, the partitioned formulation offers the further advantage of not requiring that the large matrices $D(\mathbf{y})$ and $[\mathbf{H}^T D^{-1}(\mathbf{y})\,\mathbf{H}]$ actually possess inverses.

Conclusion

In view of the clear minimum-variance basis, and the reduced matrix inversion requirements relative to solving the Normal equations, one can forsee the future use of partitioned least squares, especially Eqs. (13)-(15), in a wide variety of data-evaluation applications.

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