

## Accuracy Limitations in an Unbiased Optimum Data Treatment

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Simple explicit formulas are derived for an evaluation of the elements of the covariance matrix needed for the calculation of statistical errors which arise when some optimum linear estimates of some parameters are to be obtained from experimental data. The considered linear estimates are of the Neumann–David type, which represents a generalization of the least squares estimate. These formulas are related to the case of polynomial nonrandom data components with a stationary random component, the correlation function of which may be approximated by an exponential function. The results of this paper can be used during the design stage of the preparation of an experiment for the choice of parameters of experimental facility, such as the observing interval, number of experimental points, etc., as the formulas characterizing errors in results of data treatment are functions of these parameters.

### 1. THE NEUMANN–DAVID ESTIMATE

Let us consider an  $(n + 1)$ -dimensional data vector  $\mathbf{y}$ ,

$$\mathbf{y} = X\mathbf{a} + \overset{\dagger}{\mathbf{x}}, \quad (1)$$

where  $X$  is an  $(n + 1) \times m$  full rank nonrandom matrix,  $\mathbf{a}$  is an unknown  $m \times 1$  nonrandom vector, and  $\overset{\dagger}{\mathbf{x}}$  is an  $(n + 1) \times 1$  random vector representing some statistical errors, noise, etc.

The result  $z$  of a linear transformation  $\mathcal{L}\{\mathbf{y}\}$  of the data vector  $\mathbf{y}$  is to be determined,

$$z = \mathcal{L}\{\mathbf{y}\}. \quad (2)$$

An exact determination of the result  $z$  is impossible because of the presence of random component  $\overset{\dagger}{\mathbf{x}}$ . Therefore, a linear estimate  $\tilde{z}$ ,

$$\tilde{z} = \mathbf{w} \cdot \mathbf{y}, \quad (3)$$

using an estimator  $\mathbf{w}$ , is sought. A mean  $E\{\mathbf{x}^+\}$  of the random component  $\mathbf{x}^+$  can be included into the component  $X\mathbf{a}$ . One can therefore suppose

$$E\{\mathbf{x}^+\} = 0, \quad (4)$$

where the symbol  $E\{\cdot\}$  denotes the mathematical expectation. If the unbiasedness of the estimate  $\tilde{z}$  is required,

$$E\{\tilde{z}\} = 0, \quad (5)$$

then the following equation should hold:

$$\mathbf{w} \cdot X = \mathbf{p}, \quad (6)$$

where the  $1 \times m$  nonrandom vector  $\mathbf{p}$  characterizes the operation to be performed on the nonrandom component of the data vector,

$$\mathcal{L}\{X\mathbf{a}\} = \mathcal{L}\{X\}\mathbf{a} = \mathbf{p} \cdot \mathbf{a} \quad (7)$$

for an arbitrary vector  $\mathbf{a}$ .

It follows from the Neumann–David theorem [1] that among all linear unbiased estimates, the estimate

$$\tilde{z} = \mathbf{p}(X^T B^{-1} X)^{-1} X^T B^{-1} \mathbf{y} \quad (8)$$

has a minimum variance equaling

$$D_z = \mathbf{p}(X^T B^{-1} X)^{-1} \mathbf{p}^T, \quad (9)$$

where the  $(n + 1) \times (n + 1)$  matrix  $B$  is a diagonal matrix having on the main diagonal the variances of individual components of the data vector. Such a model comes into consideration if these components are mutually uncorrelated. A generalization of the Neumann–David theorem is given in Ref. [2] covering all possible cases of unbiased linear estimates, including a more general model of data vector (1). As shown in Ref. [2], a more general definition of the matrix  $B$  appearing in Eqs. (8) and (9) can be used,

$$B = E\{\mathbf{x}^+ \mathbf{x}^+\}, \quad (10)$$

being valid also for correlated components of the random vector  $\mathbf{x}^+$ .

As follows from the optimality of the Neumann–David estimate, no linear data handling process exists satisfying the constraint (6) of unbiasedness and giving an estimating error less than  $D_z$ . Thus Eq. (9) represents an accuracy limit for the given problem.

Let us define a special type of linear operation defined as

$$p_s = \| d_{s-1} ; d_{s-2} ; \dots d_{s-m} \|, \tag{11}$$

where

$$d_r = \begin{cases} 1 & \text{for } r = 0, \\ 0 & \text{for } r \neq 0. \end{cases} \tag{12}$$

In this case, an estimate  $\tilde{a}_s$  of the component  $a_s$  of the vector  $\mathbf{a}$  can be obtained. Combining the estimates  $\tilde{a}_s$  for all  $s = 1, \dots, m$  into a vector  $\tilde{\mathbf{a}}$  one obtains the vector estimate

$$\tilde{\mathbf{a}} = (X^T B^{-1} X)^{-1} X^T B^{-1} \mathbf{y}, \tag{13}$$

which is the well-known Gauss–Markov estimate.

The covariance matrix of this estimate follows from Eq. (9):

$$H = G^{-1} = [E\{\tilde{\mathbf{a}} \cdot \tilde{\mathbf{a}}^T\}]^{-1} = [X^T B^{-1} X]^{-1}. \tag{14}$$

Conversely, if the covariance matrix (14) of the Gauss–Markov estimate is available, then the variance (9) of a Neumann–David estimate for an arbitrary type of linear operation can be easily determined. It is the aim of this paper to evaluate the elements of the covariance matrix (14) for some important practical cases.

## 2. INVERSION OF THE COVARIANCE MATRIX

### 2.1. Polynomial Base

The matrix  $X$  defines a base of a subspace of the  $(n + 1)$ -dimensional vector space occupied by data vectors [2]. We shall consider the often occurring special case of the polynomial base with uniformly distributed nodes, for which the element of the matrix  $X$  is

$$x_{sj} = (st_0)^{j-1}, \quad (s = 0, 1, \dots, n \quad j = 1, 2, \dots, m), \tag{15}$$

where  $t_0$  is a given positive constant. For  $n \geq m$  the rank of matrix  $X$  is  $m$ . We suppose the regularity of the matrix  $B$ . Then the inverse matrix  $G^{-1}$  exists at least theoretically. Unfortunately, it is not easy to calculate this inverse for cases which have a large value for the parameter  $m$  and which have a great number of nodes. In such cases, the order of magnitude of smallest and greatest absolute values of

elements of the matrix  $G$  differ in such a degree that the ordinary word length of a computer can be insufficient for the inversion procedure. Also, for a great number of nodes, the high requirements as to the memory and operational time of a computer involve difficulties. On the other hand, it is often interesting to have at least an estimate of the inverse matrix in an analytical form as it can be useful for the consideration of the statistical errors of the optimum data treatment or for the variance analysis. Thus, there are reasons for an analytical solution.

Johnson [3] has shown the approximate analytical calculation of the variance of the optimum discrete filter output for the uncorrelated case. It will be shown below that an explicit analytical approximate formula can be found for every element of the inverse matrix for the uncorrelated case, as well as for a simple but important case of correlated random component corrupting the treated data.

## 2.2. Uncorrelated Case

For an uncorrelated stationary random component having unitary variance the equation  $B = E$  (16) holds, where the matrix  $E$  is the unity matrix.

The matrix  $G$  characterized by Eqs. (14) and (15) has the following elements:

$$g_{p,r} = \sum_{s=0}^{s=n} (st_0)^{p+r-2}, \quad (17)$$

where

$$p, r = 1, 2, \dots, m.$$

Letting  $H$  denote the inverse of the matrix  $G$ , we have

$$GH = E. \quad (18)$$

This matrix equation can be written as  $m$  vector equations having the form

$$G\mathbf{h}_i = \mathbf{h}_i \cdot \mathbf{u}_i, \quad (19)$$

where the  $m$ -dimensional vector  $\mathbf{h}_i$  represents the  $i$ -th row or column of the symmetrical inverse matrix  $H$  and where the vector  $\mathbf{u}_i$  has elements

$$u_{ji} = d_{i-j}, \quad (20)$$

with the same  $d_r$  as in Eq. (12). It is reasonable to change the scale of the  $k$ -th component  $h_{ik}$  of the unknown vector  $\mathbf{h}_i$  according to the formula

$$h_{ik} = f_{ik}/(nt_0)^k, \quad (21)$$

and to divide the  $s$ -th equation of the system (19) by the number  $(nt_0)^{s-1}$ . The resulting system is

$$\begin{aligned}
 (g_{11}/(nt_0)^1)f_{i1} + \dots + (g_{1m}/(nt_0)^m)f_{im} &= 0 \\
 \dots \quad \dots \quad \dots &= 0 \\
 (g_{i1}/(nt_0)^i)f_{i1} + \dots + (g_{im}/(nt_0)^{i+m-1})f_{im} &= 1/(nt_0)^{i-1} \\
 \dots \quad \dots \quad \dots &= 0 \\
 (g_{m1}/(nt_0)^m)f_{i1} + \dots + (g_{mm}/(nt_0)^{2m-1})f_{im} &= 0,
 \end{aligned} \tag{22}$$

where

$$i = 1, \dots, m.$$

It is well-known that

$$\sum_{s=0}^n s^q = \begin{cases} n + 1 & \text{for } q = 0, \\ \frac{n^{q+1}}{(q+1)} + \frac{n^q}{2} + \frac{qn^{q-1}}{12} - \frac{q(q-1)(q-2)}{720}n^{q-3} \dots & \text{for } q \neq 0. \end{cases} \tag{23}$$

For a particular value  $q$ , the term containing  $n^0$  is to be omitted, the last term of the series contains  $n^1$  or  $n^2$ . Therefore,

$$\lim_{n \rightarrow \infty} (g_{pr}/(nt_0)^{p+r-1}) = 1/(t_0(p+r-1)). \tag{24}$$

Thus, for a sufficiently great number of nodes the following system of approximate equations holds:

$$\begin{aligned}
 f_{i1}/1 + \dots + f_{im}/m &= 0 \\
 \dots \quad \dots \quad \dots &= 0 \\
 f_{i1}/i + \dots + f_{im}/(m+i-1) &= t_0/(nt_0)^{i-1} \\
 \dots \quad \dots \quad \dots &= 0 \\
 f_{i1}/m + \dots + f_{im}/(2m-1) &= 0.
 \end{aligned} \tag{25}$$

This system of equations can be solved using an idea similar to that used in calculating the orthogonal polynomials [4]. The sum of the terms in the  $s$ -th equation would be

$$f_{i1}(s) + f_{i2}(s+1) + \dots + f_{im}(s+m-1) = Q_s/(s(s+1) \dots (s+m-1)), \tag{26}$$

where

$$Q_s = \begin{cases} 0 & \text{for } s \neq i, \\ t_0(m+i-1)!/(nt_0)^{i-1}(i-1)! & \text{for } s = i. \end{cases} \quad (27)$$

The condition (27) will be satisfied by the quotient  $Q_s$  having the following form:

$$Q_s = \frac{t_0}{(nt_0)^{i-1}} \frac{(m+i-1)!}{(i-1)!} \frac{(s-1)(s-2) \cdots (s-i+1)(s-i-1) \cdots (s-m)}{(i-1)(i-2) \cdots (+1)(-1) \cdots (i-m)}.$$

Multiplying Eq. (26) by the factorial  $(m+s-1)!$  and substituting

$$s+k-1=0 \quad (28)$$

we get

$$\tilde{h}_{ik} = \frac{t_0}{(nt_0)^{i+k-1}} \frac{(-1)^{i+k-2} (m+i-1)! (m+k-1)!}{(i+k-1)(m-k)! (m-i)! [(k-1)!(i-1)!]^2}. \quad (29)$$

The expression (29) is the first approximation to the actual value  $h_{ik}$ . It is valid only for a sufficiently great number of nodes  $n$ . The absolute value of the approximation error decreases with  $n$  increasing. A second approximation for the uncorrelated case can be obtained as a special case from Eq. (37) of the correlated case.

### 2.3. Correlated Case

If the corrupting random components of the treated data are correlated and if the correlation between two components  $\tilde{x}_i$  and  $\tilde{x}_{i+\tau}$  can be approximated by the function

$$E\{\tilde{x}_i \tilde{x}_{i+\tau}\} = k_0^2 \exp(-\tau/T), \quad (30)$$

where  $T$  is a positive constant, then the covariance matrix  $B$  can be shown to have the elements

$$b_{ij} = k_0^2 q^{|i-j|} \quad (i, j = 0, 1, \dots, n), \quad (31)$$

where

$$q = \exp(-t_0/T), \quad (32)$$

the positive constant  $t_0$  being the same as in Eq. (15). Equation (31) is valid for a regular distribution of nodes, i.e., when Eq. (15) holds. The inversion of this covariance matrix can be performed analytically and the element  $b_{ij}$  of the inverse matrix  $B^{-1}$  can be calculated [5] according to the formulas

$$b_{ij}^+ = \begin{cases} 1 + q^2(1 - d_{i(n-i)})/k_0^2(1 - q^2) & \text{for } i = j, \\ -q/k_0^2(1 - q^2) & \text{for } |i - j| = 1, \\ 0 & \text{for } |i - j| > 1. \end{cases} \quad (33)$$

In this case, an element of the matrix (14) can be written in the form

$$\begin{aligned}
 g_{p,r} = & t_0^{p+r-2} k_0^{-2} (1 - q^2)^{-1} \left\{ (1 + q^2) \sum_{i=0}^{i=n} i^{p+r-2} \right. \\
 & - q^2 (n^{p+r-2} + d_{p+r-2}) - q \sum_{i=0}^{i=n} [(i - 1)^{p-1} i^{r-1} \\
 & \left. + i^{p-1} (i - 1)^{r-1}] + q [(-1)^{p-1} d_{r-1} + (-1)^{r-1} d_{p-1}] \right\}.
 \end{aligned}
 \tag{34}$$

Using Eq. (23) again and neglecting all terms of the order  $1/n^2$  and higher, one obtains an approximation valid for a large value  $n$ ,

$$g_{p,r} / (nt_0)^{p+r-1} = k_0^{-2} (nt_0)^{-1} \{ c / (p + r - 1) + d_{p+r-2} + 1 \} / 2,
 \tag{35}$$

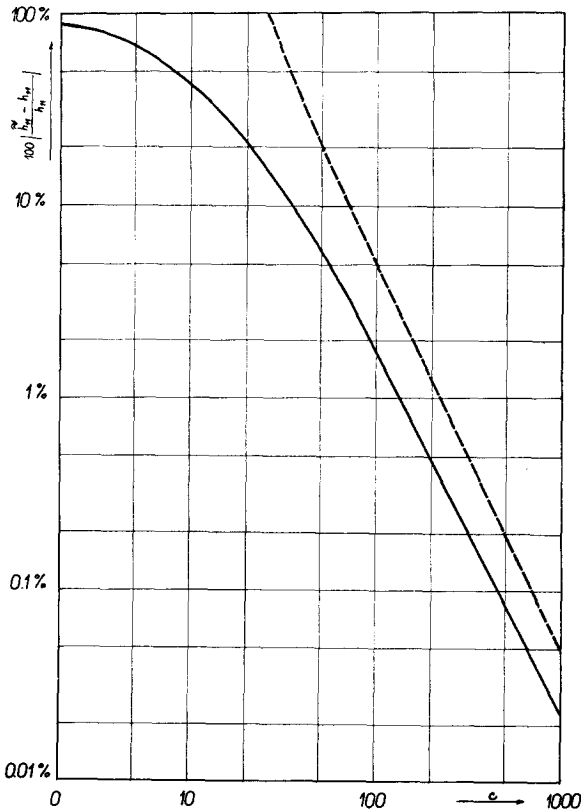


FIG. 1. The relative errors of the approximating formulas (37), (full line) and (40) (dashed line), for the case  $m = 5, p = r = 1$ .

where

$$c = 2n(1 - q)/(1 + q) = 2n[1 - \exp(-t_0/T)]/[1 + \exp(-t_0/T)]. \tag{36}$$

Solving Eq. (18) where the elements of the matrix  $G$  have the form (35) one gets the second approximation to the element  $h_{pr}$  for the correlated case,

$$\tilde{h}_{pr} \approx 2k_0^2(nt_0)^{-(p+r-2)}[a_{pr} - a_{p1}a_{r1}/(c + a_{11})]/c, \tag{37}$$

where

$$a_{pr} = \tilde{h}_{pr} - \left( \sum_{i=1}^{i=m} \tilde{h}_{pi} \right) \left( \sum_{j=1}^{j=m} \tilde{h}_{rj} \right) / \left( c + \sum_{i,j=1}^{i,j=m} \tilde{h}_{ij} \right). \tag{38}$$

It is obvious from Eq. (35) that the error of the approximation (38) for a great value  $n$  will be a function of the parameter  $c$ . Such dependence is shown in Fig. 1 by the full line for the case  $m = 5, p = r = 1$ .

### 3. APPLICATION

The quantity  $T$  in Eq. (30) is a characteristic of a physical object and as a rule it cannot be modified by an experimenter. But the quantities  $t_0$  and  $n$  are important parameters closely connected with the hardware of an experimental facility and their choice influences the economy of an experiment. The approximate formulas mentioned above may be of help for designing an experiment.

#### 3.1. Fixed interval between nodes

Let us consider both parameters  $t_0$  and  $T$  as equal to given constants. Defining another constant

$$c_1 = 2[1 - \exp(-t_0/T)]/[1 + \exp(-t_0/T)], \tag{39}$$

and considering a case with a sufficiently high value  $n$ , one obtains from Eqs. (37) and (38) a simple formula

$$\begin{aligned} \tilde{h}_{pr} \approx & 2k_0^2(nt_0)^{-(p+r-2)} \left\{ \tilde{h}_{pr}/c_1n \right. \\ & \left. - \left[ \left( \sum_{i=1}^{i=m} \tilde{h}_{pi} \right) \left( \sum_{i=1}^{i=m} \tilde{h}_{ri} \right) + \tilde{h}_{p1}\tilde{h}_{r1} \right] / c_1^2n^2 \right\}. \end{aligned} \tag{40}$$

The relative error of this approximation is demonstrated in Fig. 1 by the dashed line for the same case as above and for

$$c = c_1n. \tag{41}$$



The quantity

$$T_0 = nt_0 \quad (42)$$

may be called "the observation interval." Any increase in this quantity is undesirable as a rule because of the waste in time or in the increased size of the experimental facility. The increasing  $n$  in itself has some negative consequences as the volume of experimental work becomes greater and the treatment requires greater capacity of the computer. Thus, the increasing  $n$  in Eq. (37) or (40) improves the accuracy of the data handling results but involves other difficulties.

### 3.2. Weak correlation

For a fixed value  $n$  one gets from Eq. (36) a limit

$$\lim_{T_0/T \rightarrow \infty} c = 2n. \quad (43)$$

This case may be characterized as a weak correlation of the data vector components. It follows from Eq. (43) that for a fixed number of experimental points an increase in the observation interval brings only a limited effect in the errors of the results of the data treatment. The limit (43) corresponds to an uncorrelated case.

### 3.3. Accuracy limitations for a fixed observation interval

Let us consider the case with a constant value of the observation interval  $T_0$ . In this case, the interval  $t_0$  decreases with an increasing number of experimental points (see Eq. (42)) so that

$$\lim_{n \rightarrow \infty} c = T_0/T. \quad (44)$$

Substituting this ratio into Eq. (37) one obtains the limit values of the elements of the covariance matrix. This case corresponds to an unlimited density of experimental points within a given observation interval. In this case, all information contained in the observed part of the experimental curve is used to improve the accuracy of data treatment results. There are always practical limitations related to this density such as the dead time of detector or measuring channels, the finite size of detectors, etc. In this case, Eq. (44) together with Eq. (37) can be used for determining a reasonable compromise in choosing the parameter  $n$ .

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