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LEAST SQUARES ADJUSTMENT AND COLLOCATION

Summary

For the estimation of parameters in linear models best linear unbiased estimates are derived in case the parameters are random variables. If their expected values are unknown, the well known formulas of least squares adjustment are obtained. If the expected values of the parameters are known, least squares collocation, prediction and filtering are derived. Hence in case of the determination of parameters, a least squares adjustment must precede a collocation because otherwise the collocation gives biased estimates. Since the collocation can be shown to be equivalent to a special case of the least squares adjustment, the variance of unit weight can be estimated for the collocation also. This estimate gives the scale factor for the covariance matrices being used in the collocation. In addition, the methods of testing hypotheses and establishing confidence intervals for the parameters of the least squares adjustment may be applied to the collocation.

1. Introduction

Least squares methods of interpolation and prediction, which in a generalized form are called collocation, can be developed from the methods for the filtering and prediction of continuous signals developed in the theory of stochastic processes. However, since the collocation is always applied to discrete data, the connection of the collocation with the methods of statistics for the estimation of parameters are much closer than with stochastic processes. In fact, collocation is often obtained by means of the least squares adjustment of condition equations with parameters.

The appropriate model for the derivation of the collocation, however, is the estimation of parameters in a linear model where the parameters are random variables. By means of this model it will be shown that the collocation and the least squares adjustment are closely related. Hence, the distinct restrictions for the application of the collocation become evident. Furthermore, the statistical tests developed for the parameters in a least squares adjustment can be applied to the collocation. For these tests the variance of unit weight will be derived. Up to now, this estimate has been overlooked in connection with the collocation, although it can be used to get additional information about the covariance matrices being applied for the collocation.

Bull. Geod. 51 (1977) pp. 127–135.

2. Least Squares Adjustment for Parameters which are Random Variables

The linear model for parameters being random variables is given by [Rao. 1965, p. 192; Lewis and Odell, 1971, p. 62]

$$E(\underline{l}) = \underline{A}E(\underline{x}) \quad \text{with} \quad E(\underline{x}) = \underline{\mu}_x \tag{1}$$

where E denotes the expected value, the first moment of the random variable, $\underline{l}$ the $n \times 1$ random vector of observations, $\underline{A}$ the $n \times u$ known design matrix with rank $r(\underline{A}) = u$, $\underline{x}$ the $u \times 1$ random vector of unknown parameters and $\underline{\mu}_x$ its expected value. Let $n > u$, so that the system of linear equations $\underline{A}\underline{x} = \underline{l}$ is inconsistent. By adding the $n \times 1$ vector $\underline{e}$ of errors it becomes consistent.

Hence $\underline{A}\underline{x} = \underline{l} + \underline{e}$ with $E(\underline{e}) = \underline{o}$ from (1). Let

$$D(\underline{e}) = \underline{C}_{ee} \quad \text{and} \quad D(\underline{x}) = \underline{C}_{xx} \tag{2}$$

where D denotes the dispersion, the operator leading to the variances and covariances, $\underline{C}_{ee}$ the $n \times n$ nonsingular covariance matrix of $\underline{e}$ and $\underline{C}_{xx}$ the $u \times u$ nonsingular covariance matrix of $\underline{x}$. The random vectors $\underline{e}$ and $\underline{x}$ are assumed to be independent so that the $n \times n$ covariance matrix $\underline{C}_{ll}$ of the observations $\underline{l}$ follows as

$$\begin{aligned} \underline{C}_{ll} &= E((\underline{l} - E(\underline{l}))(\underline{l} - E(\underline{l}))^T) \\ &= E((\underline{A}\underline{x} - \underline{e} - \underline{A}\underline{\mu}_x)(\underline{A}(\underline{x} - \underline{\mu}_x) - \underline{e})^T) \\ &= \underline{A}\underline{C}_{xx}\underline{A}^T + \underline{C}_{ee} \end{aligned} \tag{3}$$

With $\underline{C}_{ss} = \underline{A}\underline{C}_{xx}\underline{A}^T$ where $\underline{C}_{ss}$ can be interpreted as the $n \times n$ covariance matrix of the vector $\underline{s}$ with $\underline{s} = \underline{A}\underline{x}$, we obtain

$$\underline{C}_{ll} = \underline{C}_{ss} + \underline{C}_{ee} \tag{4}$$

The $n \times u$ covariance matrix $\underline{C}_{lx}$ between $\underline{l}$ and $\underline{x}$ is given by

$$\begin{aligned} \underline{C}_{lx} &= E((\underline{A}(\underline{x} - \underline{\mu}_x) - \underline{e})(\underline{x} - \underline{\mu}_x)^T) \\ &= \underline{A}\underline{C}_{xx} \end{aligned} \tag{5}$$

To estimate linear functions of the parameters and the parameters themselves, the method of the best linear unbiased estimate (BLUE) is applied [Rao, 1965, p. 192]. This means, the linear function $\underline{a}^T\underline{x}$ shall be estimated by $\underline{b}^T\underline{l} + c$, where $\underline{a}$ is a given $u \times 1$ vector, $\underline{b}$ an unknown $n \times 1$ vector and c an unknown constant, which has to be added in order to fulfill (1), since both $\underline{l}$ and $\underline{x}$ are random variables. The unknown quantities $\underline{b}$ and c are determined by the conditions

$$E(\underline{b}^T\underline{l} + c) = E(\underline{a}^T\underline{x}) \tag{6}$$

and

$$V(\underline{b}^T\underline{1} + c - \underline{a}^T\underline{x}) \rightarrow Min \tag{7}$$

where V denotes the variance.

First it is assumed as usual that the expected values $\underline{\mu}_x$ of the parameters $\underline{x}$ are unknown. From (6) we get

$(\underline{a}^T - \underline{b}^T\underline{A})\,\underline{\mu}_x - c = 0$ which is fulfilled for any $\underline{\mu}_x$ if

$\underline{b}^T\underline{A} = \underline{a}^T$ and $c = 0$

With these conditions we find

$$\begin{aligned} V(\underline{b}^T\underline{1} - \underline{a}^T\underline{x}) &= E\,((\underline{b}^T\underline{1} - \underline{a}^T\underline{x})(\underline{b}^T\underline{1} - \underline{a}^T\underline{x})^T) \\ &= E\,((\underline{b}^T(\underline{A}\underline{x} - \underline{e}) - \underline{a}^T\underline{x})(-\underline{b}^T\underline{e})^T) \\ &= \underline{b}^T\underline{C}_{ee}\underline{b} \end{aligned}$$

If we minimize $\underline{b}^T\underline{C}_{ee}\underline{b}$ subject to the condition $\underline{b}^T\underline{A} = \underline{a}^T$ [Koch, 1975, p. 32], we find

$$\hat{\underline{x}} = (\underline{A}^T\underline{C}_{ee}^{-1}\underline{A})^{-1}\underline{A}^T\underline{C}_{ee}^{-1}\,\underline{1} \quad \text{with} \quad D(\hat{\underline{x}}) = (\underline{A}^T\underline{C}_{ee}^{-1}\underline{A})^{-1} \tag{8}$$

The same result is obtained for the best linear unbiased estimate or the least squares adjustment in the Gauss–Markov model $E(\underline{1}) = \underline{A}\underline{x}$ where $\underline{x}$ contains fixed parameters and where $\underline{C}_{ee} = \underline{C}_{ll}$ [Wolf, 1975]. Hence, the parameters may be regarded as fixed or random, if their expected values are unknown, the formula (8) of the least squares adjustment is obtained.

3. Least Squares Collocation

Now we deal with the special case, that the parameters $\underline{x}$ are estimated, although their expected values $\underline{\mu}_x$ are known. From (6) we obtain

$$\underline{a}^T\underline{\mu}_x - \underline{b}^T\underline{\mu}_l - c = 0 \tag{9}$$

where $\underline{\mu}_l$ is the expected value of $\underline{1}$ with

$$\underline{\mu}_l = \underline{A}\underline{\mu}_x \tag{10}$$

from (1). Hence

$$\begin{aligned} V(\underline{b}^T\underline{1} + c - \underline{a}^T\underline{x}) &= E\,((\underline{b}^T\underline{1} + c - \underline{a}^T\underline{x})(\underline{b}^T\underline{1} + c - \underline{a}^T\underline{x})^T) \\ &= \underline{b}^T(\underline{C}_{ll} + \underline{\mu}_l\underline{\mu}_l^T)\,\underline{b} - 2\underline{b}^T(\underline{C}_{lx} + \underline{\mu}_l\underline{\mu}_x^T)\,\underline{a} \\ &\quad + c^2 + 2c\underline{\mu}_l^T\underline{b} - 2c\underline{\mu}_x^T\underline{a} + a^T(\underline{C}_{xx} + \underline{\mu}_x\underline{\mu}_x^T)\,\underline{a} \end{aligned} \tag{11}$$

To minimize (11) under the constraint (9), Lagrange's function is formed by subtracting

(9) multiplied by $2k$ from (11), where k is the correlate. Differentiation with respect to $\underline{b}$, c and k and setting the results equal to zero leads to the equations

$$2(\underline{C}_{ll} + \underline{\mu}_l \underline{\mu}_l^T)\underline{b} - 2(\underline{C}_{lx} + \underline{\mu}_l \underline{\mu}_x^T)\underline{a} + 2c\underline{\mu}_l = \underline{0}$$

$$2c + 2\underline{\mu}_l^T \underline{b} - 2\underline{\mu}_x^T \underline{a} + 2k = 0$$

$$2\underline{a}^T \underline{\mu}_x - 2\underline{b}^T \underline{\mu}_l - 2c = 0$$

It follows $k = 0$, $c = \underline{\mu}_x^T \underline{a} - \underline{\mu}_l^T \underline{b}$ and $\underline{b} = \underline{C}_{ll}^{-1} \underline{C}_{lx}\underline{a}$.

Hence

$$(\text{BLUE of } \underline{a}^T\underline{x}) = \underline{a}^T\underline{\mu}_x + \underline{a}^T \underline{C}_{xl} \underline{C}_{ll}^{-1} (\underline{l} - \underline{\mu}_l)$$

and therefore with (BLUE of $\underline{x}$) $= \hat{\underline{x}}$

$$\hat{\underline{x}} = \underline{\mu}_x + \underline{C}_{xl} \underline{C}_{ll}^{-1} (\underline{l} - \underline{\mu}_l) \qquad (12)$$

This estimation is known as linear mean square regression [Cramér, 1946, p. 302 ; Wilks, 1962, p. 89]. Furthermore from (11) we get the variance of the estimation

$$V(\underline{a}^T\hat{\underline{x}} - \underline{a}^T\underline{x}) = \underline{a}^T\underline{C}_{xx}\underline{a} - \underline{a}^T\underline{C}_{xl}\underline{C}_{ll}^{-1}\underline{C}_{lx}\underline{a}$$

and therefore the covariance matrix $\underline{C}_{\hat{x}\hat{x}} = D(\hat{\underline{x}} - \underline{x})$

$$\underline{C}_{\hat{x}\hat{x}} = \underline{C}_{xx} - \underline{C}_{xl}\underline{C}_{ll}^{-1}\underline{C}_{lx} \qquad (13)$$

With $\underline{\mu}_x = \underline{0}$ we obtain from (10) $\underline{\mu}_l = \underline{0}$ and instead of (12) the well known formula of the collocation

$$\hat{\underline{x}} = \underline{C}_x \; \underline{C}_{ll}^{-1} \underline{l} \qquad (14)$$

If $\underline{x}$ and $\underline{l}$ denote different quantities, for instance geoid undulations and gravity anomalies, the application of (14) with $\underline{C}_{xl}$ and $\underline{C}_{ll}$ given is called collocation [Krarup, 1969 ; Moritz, 1972 ; Grafarend, 1976], if $\underline{x}$ and $\underline{l}$ means the same quantities at different positions or different time, (14) is called prediction, and if $\underline{x}$ and $\underline{l}$ denote the same quantity at the same position or time, (14) means filtering. To apply (13) $\underline{C}_{xx}$ must also be known.

If (14) is used with $\underline{\mu}_x \neq \underline{o}$ the estimate $\underline{x}$ is biased by $\underline{\mu}_x - \underline{C}_{xl}\underline{C}_{ll}^{-1}\underline{A}\underline{\mu}_x$ which follows from (10) and (12). If $\underline{C}_{xl}\underline{C}_{ll}^{-1}\underline{A} = \underline{I}$ where $\underline{I}$ is the unit matrix or with (3) and (5)

$$\underline{C}_{xx}\underline{A}^T(\underline{A}\underline{C}_{xx}\underline{A}^T + \underline{C}_{ee})^{-1}\underline{A} = \underline{I} \qquad (15)$$

the bias equals zero. Generally (15) will not be fulfilled so that the collocation cannot be applied if the expected values $\underline{\mu}_x$ are not known to be vanishing.

In the special case of errorless data with $\underline{C}_{ee} = \underline{0}$ and $\underline{A}$ being a $n \times n$ matrix, (15) is fulfilled so that the bias equals zero and

$$\underline{A}^{-1} = \underline{C}_{xl} \underline{C}_{ll}^{-1} \tag{16}$$

Thus, the matrix $\underline{C}_{xl}\underline{C}_{ll}^{-1}$ of transformation of the collocation (14) is inverse to the design matrix $\underline{A}$. If for instance geoid undulations have to be estimated from gravity anomalies, the inverse of Stokes' formula may be used to set up the design matrix $\underline{A}$. Thus in the special case (16) the inverse of the inverse of Stokes' formula, which is Stokes' formula itself, gives the same results as the collocation. This is true for any linear model and has been already shown for Stokes' and Molodensky's formula under the assumption that n goes to infinity by Moritz [1975].

If parameters of the gravity field shall be determined from heterogeneous data by the collocation [Moritz, 1972, p. 67], it is not sufficient in order to ensure $\underline{\mu}_x = \underline{0}$, that the sum of the parameters equal zero, as Lachapelle [1975, p. 14] assumes for the geoid undulations. The expected values of the geoid undulations of Central Europe for instance, which after referring them to the mean earth ellipsoid do not contain the effect of the zero–degree harmonic coefficient of the earth's gravity potential, are certainly different from zero. It is also not sufficient to refer the geopotential to the potential of the reference ellipsoid, in order to obtain expected values of zero for the zonal harmonic coefficients [Schwarz, 1975, p. 44]. The expected values of the zonal harmonics J_3, J_4 or J_5 minus the coefficients of the potential of the ellipsoid differ without any doubt from zero. Even if higher order reference fields are introduced instead of the ellipsoid [Rapp, 1976], the expected values of the parameters of the gravity field referred to this reference potential are still unequal to zero, so that the collocation (14) gives biased results.

In general, if the observations $\underline{l}$ contain any information about the expected values of the parameters, then $\underline{\mu}_x \neq \underline{0}$ and the least squares adjustment (8) has to be applied instead of (14) to estimate the parameters. A collocation, of course, can follow a least squares adjustment. It means that an estimate $\hat{\underline{\mu}}_x$ of $\underline{\mu}_x$ in (12) is obtained by (8)

$$\hat{\underline{\mu}}_x = (\underline{A}^T \underline{C}_{ee}^{-1} \underline{A})^{-1} \underline{A}^T \underline{C}_{ee}^{-1} \underline{l} \tag{17}$$

so that we get with (10) instead of (12)

$$\hat{\underline{x}} = \hat{\underline{\mu}}_x + \underline{C}_{xl} \underline{C}_{ll}^{-1} (\underline{l} - \underline{A}\hat{\underline{\mu}}_x) \tag{18}$$

This is the well known collocation with the inclusion of systematic terms represented by $\hat{\underline{\mu}}_x$. As mentioned, (18) describes a least squares adjustment followed by a collocation, since with

$$\hat{\bar{\underline{x}}} = \hat{\underline{x}} - \hat{\underline{\mu}}_x \quad \text{and} \quad \bar{\underline{l}} = \underline{l} - \underline{A}\hat{\underline{\mu}}_x \tag{19}$$

we obtain (14).

The collocation should be interpreted as an interpolation rather than a determination of parameters, since by substituting (19) in (18) $\hat{\underline{\mu}}_x$ may be a $k \times 1$ vector with $\hat{\underline{\bar{x}}}$ being a $u \times 1$ vector where $u > k$. If $\underline{x}$ and $\underline{1}$ denote the same quantity, one gets $\underline{\mu}_x = \underline{A}'\hat{\underline{\mu}}_x$ where the $u \times k$ matrix $\underline{A}'$ is obtained by the same model which leads to the design matrix $\underline{A}$ and which in this special application only serves to eliminate the systematic terms. Hence, we find instead of (18)

$$\hat{\underline{x}} = \underline{A}'\hat{\underline{\mu}}_x + \underline{C}_{x1}\underline{C}_{11}^{-1}(\underline{1} - \underline{A}\hat{\underline{\mu}}_x) \tag{20}$$

This is the well known formula for the least squares prediction and filtering of observations, which has been successfully applied for different kinds of interpolation (e.g. Koch [1973]).

4. Hypotheses Tests and Confidence Intervals for the Collocation

With (4) we obtain instead of the collocation (14)

$$\hat{\underline{x}} = \underline{C}_{x1}(\underline{C}_{ss} + \underline{C}_{ee})^{-1}\underline{1} \tag{21}$$

where $\underline{C}_{ss}$ and $\underline{C}_{ee}$ are assumed to be known and from (13)

$$\underline{C}_{\hat{x}\hat{x}} = \underline{C}_{xx} - \underline{C}_{x1}(\underline{C}_{ss} + \underline{C}_{ee})^{-1}\underline{C}_{1x} \tag{22}$$

To apply statistical tests to (21), we need the connection with the least squares adjustment. We consider the two cases $\underline{C}_{ee} \neq \underline{0}$ and $\underline{C}_{ee} = \underline{0}$. For the first one we get with (3) and (5) instead of (21)

$$\hat{\underline{x}} = \underline{C}_{xx}\underline{A}^T(\underline{A}\underline{C}_{xx}\underline{A}^T + \underline{C}_{ee})^{-1}\underline{1}$$

It should be mentioned that Rummel [1976] attributes this equation to Method II of the collocation and (21) to Method I by questioning the validity of the linear relationship in (1). However, without this assumption the collocation cannot be derived so that a discrimination into Method I and II is not necessary.

By means of the identity [Rao, 1965, p. 192]

$$\underline{C}_{xx}\underline{A}^T(\underline{A}\underline{C}_{xx}\underline{A}^T + \underline{C}_{ee})^{-1} = (\underline{A}^T\underline{C}_{ee}^{-1}\underline{A} + \underline{C}_{xx}^{-1})^{-1}\underline{A}^T\underline{C}_{ee}^{-1}$$

we find instead of (21)

$$\hat{\underline{x}} = (\underline{A}^T\underline{C}_{ee}^{-1}\underline{A} + \underline{C}_{xx}^{-1})^{-1}\underline{A}^T\underline{C}_{ee}^{-1}\underline{1} \tag{23}$$

and instead of (22)

$$\underline{C}_{\hat{x}\hat{x}} = (\underline{A}^T\underline{C}_{ee}^{-1}\underline{A} + \underline{C}_{xx}^{-1})^{-1} \tag{24}$$

The same results are obtained from the least squares adjustment (8)

$$\hat{\underline{x}} = (\underline{\bar{A}}^T\underline{\bar{C}}_{ee}^{-1}\underline{\bar{A}})^{-1}\underline{\bar{A}}^T\underline{\bar{C}}_{ee}^{-1}\underline{\bar{1}} \tag{25}$$

with

$$\bar{A} = \begin{vmatrix} \underline{A} \\ \underline{I} \end{vmatrix} \;,\; \bar{\underline{C}}_{ee} = \begin{vmatrix} \underline{C}_{ee} & \underline{0} \\ \underline{0} & \underline{C}_{xx} \end{vmatrix} \;,\; \bar{\underline{l}} = \begin{vmatrix} \underline{l} \\ \underline{0} \end{vmatrix}$$

where $\underline{I}$ is the $u \times u$ unit matrix and $\underline{0}$ the $u \times 1$ null vector. Thus, the collocation (21) is equivalent to the least squares adjustment where in addition to the n observations $\underline{l}$, the unknown parameters are observed as zero values with the covariance matrix $\underline{C}_{xx}$. Such a set of observations, of course, is highly unrealistic. However, it is sometimes introduced to transform an ill–conditioned system $(\underline{A}^T\underline{C}_{ee}^{-1}\underline{A})^{-1}$ into a well behaved system $(\underline{A}^T\underline{C}_{ee}^{-1}\underline{A} + \underline{C}_{xx}^{-1})^{-1}$ (e.g. Reigber and Ilk [1976]).

The estimate $\hat{\sigma}^2$ of the variance of unit weight for the least squares adjustment (25) and for the collocation (21) is given by

$$\hat{\sigma}^2 = \frac{1}{n}(\underline{l}^T\underline{C}_{ee}^{-1}\underline{l} - \hat{\underline{x}}^T\underline{C}_{\hat{x}\hat{x}}^{-1}\hat{\underline{x}}) \tag{26}$$

which can be computed by means of the covariances in (21) and (22). The estimate $\hat{\sigma}^2$ decreases with the increase of the number u of estimates $\hat{\underline{x}}$. Even if an infinite number of $\hat{\underline{x}}$ may be computed from the n observations $\underline{l}$ by (21), $\hat{\sigma}^2$ does not go to zero in a practical interpolation, since the ratio of u/n will not go beyond a certain limit.

Since $\hat{\sigma}^2$ is distributed as $\chi^2(n)$ with n degrees of freedom, the hypothesis $\sigma^2 = 1$ against $\sigma^2 > 1$ may be tested. If the hypothesis is not accepted, the covariance matrices in (21) and (22) need to be multiplied by $\hat{\sigma}^2$ so that $\hat{\underline{C}}_{\hat{x}\hat{x}} = \hat{\sigma}^2\underline{C}_{\hat{x}\hat{x}}$ gives a more realistic estimate of the covariance matrix $\underline{C}_{\hat{x}\hat{x}}$ than (22). With the knowledge of σ^2 any linear hypothesis for $\underline{x}$ may be tested, the simplest one being the t–test for one component of $\underline{x}$ [Koch, 1975, p. 53]. In addition, confidence intervals can be set up for σ^2 and $\underline{x}$.

If the observations $\underline{l}$ are errorless with $\underline{C}_{ee} = \underline{0}$, the inequality $u \geq n$ must be fulfilled in order to ensure according to (3) a nonsingular covariance matrix $\underline{C}_{ss}$. Thus, more estimates have to be computed than observations are given. They are obtained by

$$\hat{\underline{x}} = \underline{C}_{x}\;\underline{C}_{ss}^{-1}\;\underline{l} \tag{27}$$

which follows from (21) and from (22)

$$\underline{C}_{\hat{x}\hat{x}} = \underline{C}_{xx} - \underline{C}_{xl}\underline{C}_{ss}^{-1}\underline{C}_{lx} \tag{28}$$

or with (4) and (5)

$$\hat{\underline{x}} = \underline{C}_{xx}\underline{A}^T(\underline{A}\underline{C}_{xx}\underline{A}^T)^{-1}\underline{l} \tag{29}$$

and

$$\underline{C}_{\hat{x}\hat{x}} = \underline{C}_{xx} - \underline{C}_{xx}\underline{A}^T(\underline{A}\underline{C}_{xx}\underline{A}^T)^{-1}\underline{A}\underline{C}_{xx} \tag{30}$$

The results (29) and (30) are also obtained from a least squares adjustment where

$$\bar{\underline{A}} = \underline{I},\ \bar{\underline{1}} = \underline{o} \text{ and } \bar{\underline{C}}_{ee} = \underline{C}_{xx} \tag{31}$$

under the constraints

$$\underline{A}\underline{x} = \underline{1} \tag{32}$$

Hence, the estimate $\hat{\sigma}^2$ of the variance of unit weight for the collocation (27) is given by

$$\hat{\sigma}^2 = \frac{1}{u-n}\, \underline{1}^T \underline{C}_{ss}^{-1}\, \underline{1} \tag{33}$$

which will not go to zero in a practical application, since the number u of interpolated values will not surpass considerably the number n of observations.

With σ^2 given by (33) the test of the variance of unit weight, the tests of linear hypotheses and the estimates of confidence intervals mentioned above can be applied for the collocation (27).

The special case $u = n$ leading to (16) has been already mentioned in the previous chapter. We obtain instead of (27) and (28)

$$\hat{\underline{x}} = \underline{A}^{-1}\underline{1} \text{ and } \underline{C}_{\hat{x}\hat{x}} = \underline{0} \tag{34}$$

Hence, $\hat{\underline{x}}$ is determined from the constraints (32) by means of the design matrix $\underline{A}$. If the same quantities at the same positions or time are interpolated as have been measured, it follows $\underline{A} = \underline{I}$ and $\hat{\underline{x}} = \underline{1}$.

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Received : 26.08.1976
Revised : 11.01.1977