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Least Squares in Identification Theory*)

Vladimír Strejc

This article demonstrates the application of least squares for the estimation of system parameters. Analytic as well as numerical approaches are described. The model of the system dynamics is assumed in the form of regression model and in the form of discrete impulse response. Solutions are discussed for the case of white noise and correlated noise corrupting the useful output signal of the system.

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References

1. INTRODUCTION

The method of least squares was invented by a young revolutionary of his day, Karl Friedrich Gauss. He was 18 years old at the time of his first use of the least

*) The redaction of the journal intends to publish a series of survey papers on actual topics in Cybernetics. The papers should give a concise critical review on recent results in the considered field. The paper of Prof. Strejc starts this series.

Redaction.
squares method for astronomical computations in 1795. He suggested that the most appropriate values for the unknown but desired parameters are the most probable values. He defined that "the most probable value of the unknown quantities will be that in which the sum of the squares of the differences between the actually observed and the computed values multiplied by numbers that measure the degree of precision is a minimum". The difference between the observed and computed values is generally called the residual.

To make the discussion more precise, consider the following statement of the estimation problem. Suppose the identification problem. Let the mathematical model of the dynamic time invariant single input single output system be of the regressive form

\[ y(k) = \sum_{i=1}^{N} Q_i y(k - i) + \sum_{i=0}^{N} P_i u(k - i) + \epsilon(k), \]

where \( y(\cdot) \) is the output variable, \( u(\cdot) \) the input variable and \( \epsilon(k) \) represents the measurements errors that occur at each observation time \( k, k = 1, 2, \ldots, K, Q_i, i = 1, 2, \ldots, N \) and \( P_i, i = 0, 1, 2, \ldots, N \) are the weighting factors. The equation (1) can be written in the form

\[ y(k) = \mathbf{z}^T(k) \vartheta + \epsilon(k), \]

where

\[ \mathbf{z}^T(k) = [u(k - N), y(k - N), \ldots, u(k - 1), y(k - 1), u(k)], \]

\[ \vartheta^T = [P_N, Q_N, \ldots, P_0, Q_0, P_0]. \]

or in the vector-matrix form

\[ \mathbf{Y} = \mathbf{Z} \vartheta + \mathbf{E} \]

with

\[ \mathbf{Y}^T = [y(1), y(2), \ldots, y(K)], \]

\[ \mathbf{E}^T = [\epsilon(1), \epsilon(2), \ldots, \epsilon(K)] \]

and

\[ \mathbf{Z} = \begin{bmatrix} u(1 - N), & y(1 - N), & \ldots, & u(0), & y(0), & u(1) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ u(K - N), & y(K - N), & \ldots, & u(K - 1), & y(K - 1), & u(K) \end{bmatrix}. \]

For statistical and probabilistic considerations the number of observations \( K \) need to be much larger than the number \( 2N + 1 \) of parameters to be estimated in equation (1) or (2). Hence,

\[ K \gg 2N + 1. \]
In addition to the requirement (4), from equations (1) through (3) can be seen, that the measurement data and the parameters are assumed here to be linearly related, thereby making explicit the assumption about the kind i.e. linear or nonlinear procedure of estimation.

Denote the estimate of $\theta$ based on the $K$ data samples as $\hat{\theta}^* (k)$. Then the residual associated with the $k$-th measurement is

$$r(k) = y(k) - z^T(k) \hat{\theta}^*(k), \quad k = 1, 2, \ldots, K.$$  

The least squares method is concerned with determining the "most probable" value of $\theta$, that is $\hat{\theta}^*$, which is defined as the value that minimizes the sum of the squares of the residuals. Thus calculate $\hat{\theta}$ so that

$$J = \frac{1}{2} \sum_{k=1}^{K} [y(k) - z^T(k) \hat{\theta}]^T W(k)$$

is minimized. The weighting factors $W(k)$ indicate the degree of confidence that one can place in the individual measurements. In vector matrix notation, e.g. in (10), the factors $W(k)$ are arranged in weighting matrix $W$ of general quadratic form.

The sum (6) is denoted in different ways in technical literature according to the problem solved e.g. cost function, loss function, risk function, objective function etc.

In most expositions $W$ is restricted to being both symmetric positive definite although the symmetric condition is redundant, because there exist the decomposition

$$W = W_s + W_{ss},$$

where $W_s$ is symmetric and $W_{ss}$ skew-symmetric. But, since, for any nonzero column matrix $c$, $c^T W_{ss} c = 0$, it is apparent that only symmetric part $W_s$ of $W$ contributes a nonzero value to the cost function.

It is assumed that errors in the measurements expressed in equation (1) by $e(k)$ are independent of each other so the joint probability density function of measurement residuals can be expressed as the product of the individual density functions

$$f(r_1, r_2, \ldots, r_K) = f(r_1) f(r_2) \ldots f(r_K).$$

Moreover it is considered that the joint density $f(r)$ would be a normal density

$$f(r) = \sqrt{\det W} \exp \left[ -\frac{1}{2} r^T W r \right].$$

$$r^T = [r_1, r_2, \ldots, r_K].$$

In the contemporary literature dealing with estimation theory there are distinguished
mostly three different types of least squares with respect to the form of the weighting matrix $W$.

For $W$ equal to identity matrix $I$, the procedure of minimizing the sum (6) is simply called procedure of least squares. For $W$ of general form unequal zero, the denotation of weighted least squares is usual. For $W = R^{-1}$, where $R = \delta[E \ E^t]$ is the covariance matrix of the observation errors, the result is minimum variance estimate called also Markov estimate.

Although not essential to the theory, it is almost universally agreed that the linear estimates be unbiased. This restriction is equivalent to postulating that

$$\delta[E] = 0.$$  

2. ANALYTIC SOLUTION OF LEAST SQUARES

The cost function (6) for $k = 1, 2, \ldots, K$ can be expressed in the vector matrix form

$$J = \frac{1}{2}[\mathbf{Y} - \mathbf{Z}\hat{\theta}]^t W[\mathbf{Y} - \mathbf{Z}\hat{\theta}].$$

To determine the conditions that minimize the quadratic cost function (10), let us differentiate it with respect to the parameters and equate the result to zero. Thus for $W = I$ we have

$$\frac{\partial J}{\partial \hat{\theta}} = -\mathbf{Z}^t[\mathbf{Y} - \mathbf{Z}\hat{\theta}] = 0$$

and the least square estimate is

$$\hat{\theta} = (\mathbf{Z}^t\mathbf{Z})^{-1} \mathbf{Z}^t\mathbf{Y}.$$  

It can be proved (R. Deutsch [1969]) that the estimate (12) yields an absolute minimum of the quadratic cost function (10).

It is now easy to demonstrate that $\hat{\theta}$ is unbiased estimate. Consider

$$\delta[\hat{\theta} - \theta] = \delta[(\mathbf{Z}^t\mathbf{Z})^{-1} \mathbf{Z}^t\mathbf{Y}] - \theta = (\mathbf{Z}^t\mathbf{Z})^{-1} \mathbf{Z}^t \delta[\mathbf{Y}] - \theta.$$  

From equation (3) it follows that

$$\delta[\mathbf{Y}] = \mathbf{Z}\theta + \delta[E], \quad \delta[E] = 0.$$  

Hence, substituting for $\delta[\mathbf{Y}]$ in (13) we obtain finally that

$$\delta[\hat{\theta} - \theta] = 0.$$  

Therefore, $\hat{\theta}$ is an unbiased estimate.
Theorem 1. The estimate of parameters of the vector \( \beta \) in the sense of least squares is unbiased if the mean values of the components of the error vector \( E \) are equal to zero and if the measurement matrix \( Z \) and the error-vector \( E \) are mutually independent.

For the covariance matrix of the estimate \( \beta^* \) it holds:

Theorem 2. If the measurement matrix \( Z \) and the error-vector \( E \) are mutually independent, \( \delta\{E\} = 0 \), \( \delta\{EE^T\} = \sigma^2 I_K \), where \( I_K \) is the identity matrix of the dimension \( K \), and if \( \delta\{E(k) E(k-i)\} = 0 \) for \( k = 1, 2, \ldots, K \), then

\[
\delta\{(\beta^* - \beta)(\beta^* - \beta)^T\} = \sigma^2 (Z^T Z)^{-1}.
\]

Proof.

\[
\Psi_{LS} = \delta\{(\beta^* - \beta)(\beta^* - \beta)^T\} = \\
= \delta\{\beta^* \beta^T - 2 \beta^* \beta^T + \beta \beta^T\} = \\
= \delta\{\beta^* \beta^T - \beta \beta^T\} = \\
= \delta\{(Z^T Z)^{-1} Z^T \beta Y Z (Z^T Z)^{-1} \} = \\
= (Z^T Z)^{-1} Z^T \delta\{E E^T\} Z (Z^T Z)^{-1} = \\
= (Z^T Z)^{-1} Z^T \delta\{EE^T\} Z (Z^T Z)^{-1} = \sigma^2 (Z^T Z)^{-1}.
\]

It was used the fact that \( \delta \beta^* = \delta \beta \).

In a similar way for the weighted least squares the following relations may be derived:

The estimate of parameters

\[
\beta^* = (Z^T W Z)^{-1} Z^T W Y = Q Y.
\]

The covariance matrix of the estimate is

\[
\Psi_{WLS} = \delta\{(\beta^* - \beta)(\beta^* - \beta)^T\} = Q \delta\{EE^T\} Q^T,
\]

where \( Q \) follows from relation (17).

For \( W^{-1} = R = \delta\{EE^T\} \) we have the minimum variance estimate (Markov estimate)

\[
\beta^* = (Z^T R^{-1} Z)^{-1} Z^T R^{-1} Y
\]

and the covariance matrix of the minimum variance estimate

\[
\Psi_{MW} = \delta\{(\beta^* - \beta)(\beta^* - \beta)^T\} = (Z^T R^{-1} Z)^{-1}.
\]
3. RECURSIVE SOLUTION OF LEAST-SQUARES

It happens when solving practical problems that the number \( K \) of rows of the matrix \( Z \) in (3) is successively updated. Because \( K \) may be a very large number, it is uneconomical to repeat in all instants of sampling the calculation of parameters with all past measured data stored in the matrix \( Z \), namely if the number of rows was increased by one row only. Such a situation occurs when identifying the dynamic system properties on line.

For single input single output system the following denotation will be used

\[
(21) \quad Y_{k+1} = \begin{bmatrix} Y_k \\ y_{k+1} \end{bmatrix}, \quad Z_{k+1} = \begin{bmatrix} Z_k \\ z_{k+1} \end{bmatrix},
\]

where the last row of \( Z_{k+1} \) is

\[
z_{k+1} = [u(k+1-N), y(k+1-N), \ldots, u(k), y(k), u(k+1)].
\]

The least-squares estimate of parameters is according to (12)

\[
(22) \quad \hat{\theta}_{k+1} = (Z_k^T Z_k + z_{k+1} z_{k+1}^T)^{-1} Z_k^T Y_{k+1} = (Z_k^T Z_k + z_{k+1} z_{k+1}^T)^{-1} (Z_k^T Y_k + z_{k+1} y_{k+1}).
\]

Using the matrix inversion lemma, the inversed matrix on the left-hand side of (22) is

\[
(z_k z_k^T + z_{k+1} z_{k+1}^T)^{-1} = (z_k z_k^T)^{-1} - (z_k z_k^T)^{-1} z_{k+1} z_{k+1}^T (z_k z_k^T)^{-1}.
\]

Introducing

\[
(23) \quad M_k = (Z_k^T Z_k)^{-1} z_{k+1} [1 + z_{k+1} (Z_k^T Z_k)^{-1} z_{k+1}]^{-1}
\]

and noting that

\[
(24) \quad (Z_k^T Z_k)^{-1} z_{k+1} = (Z_k^T Z_k)^{-1} z_{k+1} [1 + z_{k+1} (Z_k^T Z_k)^{-1} z_{k+1}]^{-1}.
\]

it is possible to write, that

\[
(25) \quad \hat{\theta}_{k+1} = \hat{\theta}_k + M_k (y_{k+1} - z_{k+1}^T \hat{\theta}_k).
\]

It is evident that the estimate corresponding to \( k + 1 \) samples equals to the previous estimate \( \hat{\theta}_k \) corrected by the term proportional to \((y_{k+1} - z_{k+1}^T \hat{\theta}_k)\). The product \( z_{k+1}^T \hat{\theta}_k \) may be considered as the prediction of the value \( y_{k+1} \) based on the estimate of parameters \( \hat{\theta}_k \) and on the set of measurements \( z_{k+1} \). The predicted value \( \hat{y}_{k+1} = z_{k+1}^T \hat{\theta}_k \) equals to the right value \( y_{k+1} \) only if the exact system model with para-
meters $\theta_{k}^{*} = \theta_{k+1}$ is available and if the noise is absent. In such a case the correction is zero.

Elements of the matrix $M_k$ are weighting coefficients. In order to calculate $M_k$, in a recursive way, it is possible to introduce

$P(k) = x(Z^T_i Z_j)^{-1}$.

where $x$ is a positive constant. Then

$M_k = P(k) z_{k+1}[x + z_{k+1}^T P(k) z_{k+1}]^{-1}$.

Substituting the matrix $P(k)$ defined by (26) into (22), we have

$P(k+1) = P(k) - P(k) z_{k+1}[x + z_{k+1}^T P(k) z_{k+1}]^{-1} z_{k+1}^T P(k) = [I - M_k z_{k+1}^T] P(k)$.

Hence, the estimate of parameters according to least squares approach may be calculated by the following recursive formulas:

$M_k = P(k) z_{k+1}[x + z_{k+1}^T P(k) z_{k+1}]^{-1}$.

$P(k+1) = [I - M_k z_{k+1}^T] P(k)$.

$\theta_{k+1} = \theta_{k} + M_k [y_{k+1} - z_{k+1}^T \theta_{k}]$.

These formulas have a very close relation to the recursive algorithms of the Kalman’s filtration and can be easily extended for the multidimensional systems.

The details concerning the starting of the numerical calculation will not be considered here.

4. DISCRETE SQUARE ROOT FILTERING

In many practical problems of parameter estimation it arises the problem to solve an overdetermined ill conditioned set of algebraic equations. To circumvent this difficulty it is possible to apply the method for propagating the error covariance matrix in a square root form. This method is very successful in maintaining the positive semidefinite nature of the error covariance and can provide twice the effective precision of the conventional filter implementation in ill-conditioned problems. The outstanding numerical characteristics and a relative simplicity of this recursive square root approach led to its implementation in many practical applications. A survey of current techniques is described by P. G. Kaminski et al. [1971].

For the sake of generality consider the multi input multi output system the mathematical model of which is described by equation

$Y - Z \theta = E$. 
The respective cost function corresponding to the least squares may have the form

$$E\mathbf{r}_e^{-1}\mathbf{e}^T = (\mathbf{Y} - \mathbf{Z}\Theta)^{-1}(\mathbf{Y} - \mathbf{Z}\Theta)^T$$

or

$$\|E\mathbf{r}_e^{-1/2}\|^2 = \|\mathbf{e}\|^2 = \|(\mathbf{Y} - \mathbf{Z}\Theta)^{-1/2}\|^2.$$

In this particular case \(K\) is the number of linearity independent equations, \(p\) is the number of linearity independent sets of solutions, \(v\) is the number of estimated parameters in one set of solutions. The matrix \(\mathbf{E}\) is the matrix of random errors, \(\mathbf{Y}\) and \(\mathbf{Z}\) are matrices of data enabling to estimate the required parameters in the matrix \(\Theta\).

$$\mathbf{R}_e = \mathbf{E} \{\mathbf{e}(k) \mathbf{e}^T(k)\},$$

$$\mathbf{e}^T(k) = [e_1(k), e_2(k), \ldots, e_p(k)],$$

is in general the covariance matrix of the noise of the components of the vector \(y_t(k) = [y_1(k), y_2(k), \ldots, y_p(k)]\), which for \(k = 1, 2, \ldots, K\) gives the matrix \(\mathbf{Y}\).

$$\|\mathbf{E}\|^2$$ is the square of the euclidian norm i.e. the sum of squares of all elements of the matrix \(\mathbf{E}\).

$$\|\mathbf{E}\|^2 = \frac{1}{K} \sum_{k=1}^{K} \mathbf{e}^T(k) \mathbf{e}(k) = \frac{1}{K} \text{tr} \{\mathbf{E}^T\mathbf{E}\},$$

$$\mathbf{e}^T(k) = [e_1^*(k), e_2^*(k), \ldots, e_p^*(k)].$$

Let us remind that the norm of a matrix remains unchanged by orthogonal transformation because

$$\mathbf{E}^T\mathbf{T}\mathbf{T}^T\mathbf{E}^T = \mathbf{E}^T\mathbf{E} = \|\mathbf{E}\|^2$$

for \(\mathbf{T}\mathbf{T}^T = \mathbf{I}\), where \(\mathbf{T}\) is an orthogonal transformation matrix. (For advanced version see V. Peterka [1975].)

For the numerical solution it is useful to write the equation (34) in the form

$$\|\mathbf{E}\|^2 = \|\mathbf{D}\Theta^{-1}\mathbf{r}_e^{-1/2}\|^2,$$

where \(\mathbf{D} = [\mathbf{Z}, \mathbf{Y}]\) and \(\Theta^{-T} = [-\Theta, \mathbf{I}_p]\) and the index \(p\) denotes the dimension of the identity matrix \(\mathbf{I}_p\). The main idea of square root filtering is to find such an orthogonal transforming matrix \(\mathbf{T}\) in order to compress the matrix \(\mathbf{D}\) into upper triangular matrix \(\mathbf{D}_r\) of the dimension \((v + p; v + p)\) so that

$$\|\mathbf{E}\|^2 = \|\mathbf{D}_r\Theta^{-1}\mathbf{r}_e^{-1/2}\|^2 = \|\mathbf{D}_r\Theta^{-1}\mathbf{r}_e^{-1/2}\|^2.$$
The indicated transformation is performed successively by transforming matrices $T_i$, $i = 1, 2, \ldots, l$ so that

$$ T = \prod_{i=1}^{l} T_i. $$

$T_i$ may be so called matrices of elementary rotations (D. K. Faddeev, V. N. Faddeeva, [1960]) of the dimension $(v + p + 1; v + p + 1)$ and of the form

$$ T_i = \begin{pmatrix}
    1 & & & & \\
    & \ddots & & & \\
    & & 1 & & \\
    & & & \ddots & \\
    & & & & 1
\end{pmatrix}, $$

where all other elements are equal to zero. In order that the matrix $T_i$ be orthogonal, is necessary to fulfill the condition

$$ c_i^2 + s_i^2 = 1, $$

however one of the coefficients is possible to choose. When multiplying only $(v + p + 1)$ rows of the matrix $D = [d_{ij}]$ by $T_i$ and when denoting the elements of $T_i D$ by $d_{ij}$, then

$$ d_{ij}^* = \begin{cases}
    d_{ii} & \text{for } k = i, \\
    c_i d_{ii} + s_i d_{ji} & \text{for } k = i, \\
    -s_i d_{ii} + c_i d_{ji} & \text{for } k = j,
\end{cases} \quad l = 1, 2, \ldots, v + p. $$

Hence, we can choose one of the coefficients so that $d_{jj}^* = 0$, $j = 1, 2, \ldots, j - 1$. By the repetition of this procedure the upper triangular matrix of the dimension $(v + p; v + p)$ is obtained. The row $(v + p + 1)$ has all elements equal to zero. Shifting to this place the next row $(v + p + 2)$ of the original matrix $D$ it is possible to zero again all elements of this row by the described procedure and correct in this way the previous triangular matrix. The matrix $D_v$ is obtained when all rows of the original matrix $D$ are transformed into the triangular form. For the transformation of the row $v + p + l$, $l = 1, 2, \ldots, (K - v - p)$ it is necessary to apply $v + p$ transformations.

It is worth-while to mention that it is sufficient to store in the computer memory only the nonzero elements of the triangular matrix and elements of the new rows which are to be transformed. The latter ones may be just measured values. This kind of data reduction is advantageous namely when updating successively the matrix $D_v$ according to the new measurements.
The algorithm of calculation can be proposed in such a way that in the matrix (39) the row index is always \( y = v + p + 1 \) and only the column index \( i = 1, 2, \ldots, (v + p) \) is changed. Then the algorithm starts even for \( D_v = 0 \).

In order to keep the value of the elements of the matrix \( D_v \) in reasonable limits even for \( K \) increasing it is useful to reduce these elements according to the relation

\[
F = \frac{1}{\sqrt{K}} D_v
\]

where \( F \) is so called information matrix. This matrix may be divided with respect to the dimensions \( v \) and \( p \) into four fields

\[
F = \begin{pmatrix}
F_{\theta\theta}
& F_{\theta R}

0
& F_{R R}
\end{pmatrix}
\]

Matrices \( F_{\theta \theta}(v; v) \) and \( F_{R R}(p; p) \) have upper triangular form and the matrix \( F_{\theta R}(v; p) \) is rectangular.

Using (43) for the norm (38) we have

\[
\|E^*\|_2^2 = \|F^* R_c^{-1/2}\|_2^2, \quad E^* = \frac{1}{\sqrt{K}} E^*.
\]

(44)

The last equation defines two relations

\[
E^{*}_1 = (F_{\theta R} - F_{\theta \theta} \Theta) R_c^{-1/2},
\]

\[
E^{*}_2 = F_{\theta \theta} R_c^{-1/2}.
\]

For

\[
F_{\theta R} - F_{\theta \theta} \Theta = 0
\]

we have the residuals \( E^{*}_1 = 0 \). Since \( F_{\theta \theta} \) is a regular matrix, equation (47) enables to determine the required parameters

\[
\Theta^* = F_{\theta \theta}^{-1} F_{\theta R}.
\]

The calculation is very simple because \( F_{\theta \theta} \) and \( F_{\theta R}^{-1} \) have upper triangular form.

The matrix \( E^{*}_2 \) approaches to identity matrix for \( K \) limiting to infinity (T. W. Anderson [1958]). Hence, from equation (46) we have

\[
F_{\theta R} = R_c^{1/2}.
\]
i.e. the estimate of the right Cholesky's square root of the covariance matrix $R_p(p; p)$. 

\begin{equation}
R_p^{\times} = F_p^T F_p \mathbb{R} = R_p^{\times T/2} R_p^{\times 1/2}.
\end{equation}

The results (48) and (49) correspond to the maximum likelihood estimate of the matrix $\theta$ if the errors in the matrix $E^*$ are Gaussian and mutually independent.

In the case of least squares estimate of the matrix $\theta$ it is assumed that the errors are mutually independent as well but that they all have the same variance $\sigma^2$. Hence the covariance matrix $R_e$ is

\begin{equation}
R_e = \sigma^2 I_p,
\end{equation}

and

\begin{equation}
R_e^{1/2} = \sigma I_p.
\end{equation}

The information matrix (43) of the single input single output system has the following form

\begin{equation}
\begin{bmatrix}
\hat{f}_{11} & \hat{f}_{12} & \ldots & \hat{f}_{1,v+1} \\
\hat{f}_{21} & \hat{f}_{22} & \ldots & \hat{f}_{2,v+1} \\
\vdots & \vdots & \ddots & \vdots \\
\hat{f}_{v1} & \hat{f}_{v2} & \ldots & \hat{f}_{vv+1}
\end{bmatrix}
\begin{bmatrix}
\xi_{\theta} \\
\xi_{\theta^2} \\
\vdots \\
\xi_{\theta^{v+1}}
\end{bmatrix}
= \begin{bmatrix}
\xi_{\theta^2} \\
\xi_{\theta^2}^2 \\
\vdots \\
\xi_{\theta^{v+1}}^v
\end{bmatrix}
= \begin{bmatrix}
\frac{1}{K}
\end{bmatrix}
\end{equation}

where $e^*_i$, $i = 1, 2, \ldots, v + 1$ are observation errors transformed by the same orthogonal matrices $T_i$ as the matrix $D$ in relation (38) and $R_e^{1/2} = \sigma_e$ for the single input single output system. When solving (53) according to (47) it is possible to zero all residuals $e^*_i$, $i = 1, 2, \ldots, v$. It is not possible to influence the last residual $e^*_{v+1}$. Hence, in accordance with (49) a (53) we have

\begin{equation}
F_{RR} = f_{v+1,v+1} = R_e^{1/2} = \sigma_e^2.
\end{equation}

The relation (54) implies that

\begin{equation}
e^*_{v+1} = \frac{1}{\sqrt{K}}.
\end{equation}

The value of the cost function is

\begin{equation}
J_{\text{res}} = f_{v+1,v+1}^2 = \sigma_e^2.
\end{equation}

Knowing $\sigma_e^2$ from (54) it is possible to calculate the covariance matrix $V_{\theta}$ of the estimates of parameters $\theta_i$, $i = 1, 2, \ldots, v$ by means of (16).
The cost function of the multi input multi output system may have the form

\[
J_1 = \frac{1}{K} \sum_{k=1}^{K} \mathbf{e}^T(k) \mathbf{W} \mathbf{e}(k) = \frac{1}{K} \text{tr}(\mathbf{E} \mathbf{W} \mathbf{E}^T),
\]

where \( \mathbf{e}^T(k) = [e_1(k), e_2(k), \ldots, e_p(k)] \).

The minimum value of the cost function is

\[
J_{\text{min}}^1 = \left\| F_{\mathbf{R}_\mathbf{R}} \mathbf{W}^{1/2} \right\|^2.
\]

As it was mentioned before the cost function (57) is called the weighted least-squares.

For the minimum variance estimate (Markov estimate) of parameters of the multi input multi output system it is necessary to introduce in (57)

\[
\mathbf{W} = \mathbf{R}^{-1},
\]

where \( \mathbf{R} \) corresponds to (35). The minimum value of the cost function is

\[
J_{\text{min}}^2 = \left\| F_{\mathbf{R}_\mathbf{R}} \mathbf{R}^{-1/2} \right\|^2,
\]

where

\[
F_{\mathbf{R}_\mathbf{R}} \mathbf{R}^{-1/2} = \mathbf{I}_p.
\]

Hence,

\[
J_{\text{min}}^2 = p.
\]

It holds in general that

\[
J_{\text{min}}^2 < J_{\text{min}}^1.
\]

The last inequality is proved by R. Deutsch \[1969\].

The knowledge of \( F_{\mathbf{R}_\mathbf{R}} \) enables to calculate \( \mathbf{R}_c \) (50) but the covariance matrices \( \mathbf{V}_{\mathbf{W}_{\mathbf{L}} \mathbf{S}} \) and \( \mathbf{V}_{\mathbf{M}_{\mathbf{V}}} \) cannot be calculated by formulas (18) and (20) respectively. The calculation of the parameter-variances is in the multidimensional case much more difficult. For the Markov estimate it holds that

\[
\sigma^2[(\mathbf{\Theta}^* - \mathbf{\Theta})_j (\mathbf{\Theta}^* - \mathbf{\Theta})_s^T] = \frac{1}{K} F_{\mathbf{R}_{\mathbf{\Theta}\mathbf{\Theta}}}^{-1} F_{\mathbf{R}_{\mathbf{\Theta}\mathbf{\Theta}}}^{-T}.
\]

\[ j, s = 1, 2, \ldots, p. \]
5. CHOLESKY’S ALGORITHM

Instead of orthogonal transformations proposed in section 4 for the triangulization of the matrix $D$ in (37) we can use the so called Cholesky’s algorithm published for example in P. G. Kaminski et al. [1971] or in D. K. Faddeev et al. [1960].

In general any symmetric positive definite matrix $M$ of the dimension $(n; n)$ is possible to write in the factored form

\[ M = F^T F, \]

$F$ being the upper triangular matrix. It holds

\[ M_{ij} = \sum_{k=1}^{i} F_{ki} F_{kj}, \quad i \leq j \]  

and just for $i = j$

\[ M_{ii} = \sum_{k=1}^{i} F_{ki}^2 = F_{ii}^2 + \sum_{k=1}^{i-1} F_{ii}^2. \]

Hence

\[ F_{ii} = \sqrt{M_{ii} - \sum_{k=1}^{i-1} F_{ii}^2}. \]

For $j > i$ it follows from relation (66) that

\[ F_{ii} F_{ij} = M_{ij} - \sum_{k=1}^{i-1} F_{ki} F_{kj} \]

and for $M$ regular

\[ \det M = \det F^T \det F = \det F^2 = \prod_{i=1}^{n} F_{ii}^2 + 0. \]

Finally from (69) we have

\[ F_{ii} = \frac{1}{F_{ii}} (M_{ii} - \sum_{k=1}^{i-1} F_{ki} F_{kj}). \]

Relations (68) and (71) describe the Cholesky’s algorithm enabling to generate the matrix $F$ successively row by row. For $i = 1$ it holds that

\[ F_{11} = \sqrt{M_{11}} \quad \text{and} \quad F_{ij} = \frac{M_{ij}}{F_{1i}}, \]

and the next elements of the matrix $F$ are to be calculated according to (68) and (71).

For $M$ being positive semidefinite, $F_{ij} = 0$ everywhere $F_{ii} = 0$, $j > i$.

Without any doubt there are still other approaches how to triangulize the given matrix. Among different possibilities it is worth-while to mention the Householder algorithm (A. S. Householder [1964]) and the modified Gram Schmidt algorithm (A. Björck [1967]).
6. THE EXPONENTIAL FORGETTING

For some problems, like in the case of identification, the solution $\Theta^*$ represents the parameters of the mathematical model. In such kind of problems it may be useful to attach to the oldest values i.e. to values with the lowest indexes, the lowest weighting factors, in order that the newest values influence most significantly the resulting estimates of parameters. Such a requirement can be reached by exponential forgetting i.e. by multiplication of all rows of matrices $E^*$, $Y$, $Z$ in equation (34) by weighting factor $\phi^{K-k}$, $0 < \phi \leq 1$, $k = 1, 2, \ldots, K$. In equation (42) $\sqrt{K}$ is then necessary to replace by $\sqrt{x_k}$ where

$$ x_k = \sum_{i=0}^{K-1} (\phi^2)^i. $$

(72)

For $K$ increasing the value $x$ can be calculated recursively. It holds that

$$ x_{K+1} = \sum_{i=0}^{K} (\phi^2)^i = 1 + \phi^2 \sum_{i=0}^{K-1} (\phi^2)^i, $$

(73)

so that

$$ x_{K+1} = 1 + \phi^2 x_k. $$

(74)

7. EXAMPLES OF LEAST-SQUARES APPLICATIONS

There is a great number of different modifications of least squares evaluations according to the problems to be solved. In the field of identification and system parameter estimation it is possible to apply the least-squares not only in connection with the regression model of the system, the model which was used in preceding sections, but also in connection with other types of models. For the sake of illustration let us consider two other examples.

7.1. Discrete impulse response estimation for nonrandom inputs

Consider the system output expressed by convolution sum

$$ y_k = \sum_{i=0}^{m} u_{k-i} g_i + e_k, \quad k = 0, 1, 2, \ldots, $$

(75)

where $g_i$, $i = 0, 1, 2, \ldots, m$ are the ordinates of the discrete impulse response $g(k)$ and $y_k$, $u_k$, $k = 0, 1, 2, \ldots, K$ are the sequences of values of output and input variables respectively, however the input is not a random variable. The relation (75) may be written in the vector-matrix form

$$ y = Ug + e. $$

(76)
where

\[
\mathbf{y} = \begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_K \end{bmatrix}, \quad \mathbf{U} = \begin{bmatrix} u_0 & u_{-1} & \cdots & u_{-m} \\ u_1 & u_0 & \cdots & u_{-m+1} \\ \vdots & \vdots & \ddots & \vdots \\ u_m & u_{m-1} & \cdots & u_0 \end{bmatrix}, \quad \mathbf{g} = \begin{bmatrix} g_0 \\ g_1 \\ \vdots \\ g_m \end{bmatrix}, \quad \mathbf{e} = \begin{bmatrix} e_0 \\ e_1 \\ \vdots \\ e_K \end{bmatrix}, \quad K \geq m.
\]

If the ordinate \( g_0 = 0 \) then the lower bound of the sum (75) can be changed into \( i = 1 \) and the vectors and matrices of the equation (76) can be reduced to columns and fields demarcated by dashed lines. In this particular case the value \( y_j \) of the variable \( y \) does not depend on the value \( u_j \) of the variable \( u \), but it depends only on past values of the input \( u \).

Equation (76) has the same form as equation (3) and the vector \( \mathbf{g} \) of ordinates can be calculated exactly in the same way as the vector \( \mathbf{g} \) in section 4.

7.2. Discrete impulse response estimation for random inputs

It is a similar problem as that one solved in the preceding paragraph. Assuming that it is possible to determine the estimates of the autocorrelation function of the random input \( u \) and of the crosscorrelation function of the input \( u \) and output \( y \) then the problem can be treated as the solution of Wiener-Kolmogorov equation

\[
\sum_{\tau=0}^{i} g(\tau) R_{uv}(\tau - \tau) - R_{uy}(\tau) = 0.
\]

for \( \tau = 0, 1, 2, \ldots \). For \( \tau \gg 1 \), equation (77) can be expressed in the vector matrix form

\[
\begin{bmatrix} R_{uu}(0) & R_{uu}(1) & \ldots & R_{uu}(l) \\ R_{uu}(1) & R_{uu}(0) & \ldots & R_{uu}(l-1) \\ \vdots & \vdots & \ddots & \vdots \\ R_{uu}(l) & R_{uu}(l-1) & \ldots & R_{uu}(0) \end{bmatrix} \begin{bmatrix} g(0) \\ g(1) \\ \vdots \\ g(l) \end{bmatrix} - \begin{bmatrix} R_{uy}(0) \\ R_{uy}(1) \\ \vdots \\ R_{uy}(l) \end{bmatrix} = \begin{bmatrix} e(0) \\ e(1) \\ \vdots \\ e(l) \end{bmatrix}
\]

or

(79) \[ R_{uu} \mathbf{g} - R_{uy} = \mathbf{e}. \]

This is again the standard form of the overdetermined set of algebraic equations the numerical solution of which was described in section 4.
The procedure of generalized least-squares refers to the mathematical model (2) where
\[
e(k) = n(k) + \sum_{i=1}^{N} c_i n(k - i).
\]
In this case \(e(k)\) is not a white noise as it is assumed originally but the noise \(e(k)\) is derived from white noise by a filter having the same autoregressive parameters as the process. In general the noise is not white and the estimator (12) will yield biased results. The amount of this biasing has been found to be highly significant for even low noise-signal ratios on the system output. In order to remove the bias we define a weighted least-squares estimator (17). Following P. Eykhoff [1967], let the weighting matrix \(W\) has the property that
\[
W = V^T V,
\]
\(V\) being a lower triangular matrix. Using this notation, equations (10) and (17) can be written as
\[
J = \frac{1}{2}(VE)^T VE,
\]
\[
\theta^* = [(VZ)^T VZ]^{-1} (VZ)^T YY.
\]
The matrix \(V\) represents a “noise-whitening” filter; given \(n(k), k = 1, 2, \ldots\), as an input sequence, the output of that filter is white noise. If the sequence \(E_p = VE\) is uncorrelated with \(Z\), then
\[
\theta^* = [Z_p^T Z_p]^{-1} Z_p^T YY = [Z_p^T Z_p]^{-1} Z_p^T V(Z_p + E) = \theta + [Z_p^T Z_p]^{-1} Z_p^T E_p = \theta
\]
and the estimate is asymptotically unbiased. This is the case if \(E_p\) is a white noise sequence, i.e. \(V\) is a “noise-whitening” filter. This estimator coincides with the Markov estimator, where \(W = R^{-1}\), \(R\) being the covariance matrix of the noise \(e\).

When an apriori knowledge of the noise is lacking, the noise parameters \(c_i, i = 1, 2, \ldots, N\) in (80) have to be estimated first. D. W. Clarke [1967] suggested an explicit method for the off-line calculation of these parameters
\[
C^* = -(E^* E^*)^{-1} E^* e^*,
\]
where
\[
C^{*T} = [c_1^*, c_2^*, \ldots, c_N^*],\]
\[
e^{*T} = [e^*(N + 1), e^*(N + 2), \ldots, e^*(K)]; \quad \dim e^* = (K - N; 1),\]
\[
e^*(k) = y(k) - z^*(k) \delta^*_k,\]
The filtered sequences

\begin{equation}
\mathbf{u}_v(k) = u(k) + \sum_{i=1}^{N} c_i^v u(k-i)
\end{equation}

and

\begin{equation}
\mathbf{y}_v(k) = y(k) + \sum_{i=1}^{N} c_i^v y(k-i)
\end{equation}

are used for the calculation of the estimate

\begin{equation}
\mathbf{9}_v = \left[ \mathbf{Z}(\mathbf{u}_v, \mathbf{y}_v) \mathbf{Z}(\mathbf{u}_v, \mathbf{y}_v) \right]^{-1} \mathbf{Z}(\mathbf{u}_v, \mathbf{y}_v) \mathbf{Y}_v
\end{equation}

which can be considered as the first approximation of \( \mathbf{9} \) in (84). With this \( \mathbf{9}_v \), a new improved sequence \( \mathbf{e}^*(k) \) can be generated and then again a new i.e. the second approximation of \( \mathbf{9} \), etc.

Inspired by Clarke’s algorithm, a recursive method was suggested in the article by R. Hastings-James and M. W. Sage [1969] for the system model of the type

\begin{equation}
A(\zeta^{-1}) y(k) = B(\zeta^{-1}) u(k) + \frac{1}{C(\zeta^{-1})} e(k)
\end{equation}

It consists of two recursive least squares estimators combined via filtering. Introduce the notation

\begin{align*}
\mathbf{9}_1 \rightarrow & = \begin{bmatrix}
\mathbf{u}^*_1, \ldots, \mathbf{u}^*_N, \mathbf{b}^*_1, \ldots, \mathbf{b}^*_N
\end{bmatrix} = [\mathbf{A}^*, \mathbf{B}^*], \\
\mathbf{9}_2 \rightarrow & = \begin{bmatrix}
\mathbf{c}^*_1, \ldots, \mathbf{c}^*_N
\end{bmatrix} = \mathbf{C}^*, \\
\zeta^{-1} y(k) & = y(k-1), \\
A(\zeta^{-1}) y(k) & = y(k) + a_1^* y(k-1) + \ldots + a_N^* y(k-N), \\
B(\zeta^{-1}) u(k) & = b_1^* u(k-1) + \ldots + b_N^* u(k-N), \\
\phi_1(k) & = [-C(\zeta^{-1}) y(k-1), \ldots, -C(\zeta^{-1}) y(k-N), C(\zeta^{-1}) u(k-1), \ldots, C(\zeta^{-1}) u(k-N)], \\
\phi_2(k) & = [-e^*(k-1), \ldots, -e^*(k-N)], \\
e^*(k) & = A^*(\zeta^{-1}) y(k) - B^*(\zeta^{-1}) u(k).
\end{align*}

Note that the degree of polynomials \( A^*, B^* \) and \( C^* \) need not be necessarily the same. Unequality of the degrees of these polynomials does not introduce any changes in the
described algorithms. This note holds for all other following polynomials of the same kind. The algorithm can be written as

\[ \tilde{y}_i(k + 1) = \tilde{y}_i(k) + M_1(k + 1) e_i(k + 1), \]
\[ M_1(k + 1) = \frac{P_1(k) \phi_1(k + 1)}{1 + \phi_1^2(k + 1) P_1(k) \phi_1(k + 1)}, \]
\[ P_1(k + 1) = P_1(k) - M_1(k + 1) \phi_1^2(k + 1) P_1(k), \]
\[ e_i(k + 1) = C^r(\xi^{-1}) y(k + 1) - \phi_1^2(k + 1) \tilde{y}_i(k), \]
\[ \tilde{y}_2(k + 1) = \tilde{y}_2(k) + M_2(k + 1) e_i(k + 1), \]
\[ M_2(k + 1) = \frac{P_2(k) \phi_2(k + 1)}{1 + \phi_2^2(k + 1) P_2(k) \phi_2(k + 1)}, \]
\[ P_2(k + 1) = P_2(k) - M_2(k + 1) \phi_2^2(k + 1) P_2(k), \]
\[ e_2(k + 1) = e_2^*(k + 1) - \phi_2^2(k + 1) \tilde{y}_2(k). \]

In the computations for \( \tilde{y}_i(k + 1) \) the polynomial \( C^r(\xi^{-1}) \) is required. It is obtained via the estimate \( \tilde{y}_i(k) \).

For the generalized least squares the parameter estimates will converge to the true values if the signal-to-noise ratio is large enough. On the other hand, if this ratio is small, it is possible that the estimator converge to false values.

9. INSTRUMENTAL VARIABLE METHOD

An off-line estimator which will always give asymptotically unbiased estimates is the instrumental variable method. The basic idea, see e.g. M. G. Kendall and A Stuart [1961], is the generation of an extra signal, i.e. the instrumental variable, which is correlated with the useful signal of the process but which is uncorrelated with the noise.

Introduce

\[ \psi^* = [X^\pi Z]^{-1} X Y, \]

where \( Z \) may have the form

\[ Z = \begin{bmatrix} \phi^T(1) \\ \vdots \\ \phi^T(K) \end{bmatrix}, \]
\[ Y = \begin{bmatrix} y(1) \\ \vdots \\ y(K) \end{bmatrix}, \]

\[ \phi^T(k) = [-y(k - 1), \ldots, -y(k - N), u(k - 1), \ldots, u(k - N)] \]
and

\( \mathcal{X} = \begin{bmatrix} x^T(1) \\ \vdots \\ x^T(K) \end{bmatrix} \),

\[ x^T(k) = \left[ - \frac{B(\xi^{-1})}{A(\zeta^{-1})} u(k - 1), \ldots, - \frac{B(\xi^{-1})}{A(\zeta^{-1})} u(k - N), u(k - 1), \ldots, u(k - N) \right]. \]

\( \mathcal{X} \) is called the instrumental matrix if the following two conditions are fulfilled:

\begin{align*}
\lim_{k \to \infty} \frac{1}{K} \mathcal{X}^T Z & = R, \\
\lim_{k \to \infty} \frac{1}{K} \mathcal{X}^T (Y - Z \mathcal{X}^*) & = 0,
\end{align*}

i.e. the probability limit of the sequence is non-singular (quadratic) matrix and

\[ Y - Z \mathcal{X} = \epsilon. \]

Matrix \( \mathcal{X} \) defined by relations (100) meet the assumptions (101) and (102) for open loop operation only. Note that the matrix \( \mathcal{X} \) is formed like the matrix \( Z \) but the values of the output variable are suggested without noise. The instrumental variable estimate (98) can be modified into an equivalent recursive algorithm of the form

\begin{align*}
\mathcal{X}^*(k + 1) & = \mathcal{X}^*(k) + M(k + 1) \epsilon(k + 1), \\
M(k + 1) & = \frac{P(k) \phi(k + 1)}{1 + \phi^2(k + 1) P(k) \phi(k + 1)}, \\
P(k + 1) & = P(k) - \frac{P(k) \phi(k + 1) P(k)}{1 + \phi^2(k + 1) P(k) \phi(k + 1)} = [I - M(k + 1) \phi^2(k + 1)] P(k), \\
\epsilon(k + 1) & = \gamma(k + 1) - \phi^T(k + 1) \mathcal{X}^*(k).
\end{align*}

It is evident from (100) that \( A(\zeta^{-1}) \) and \( B(\xi^{-1}) \) are required for the calculation of \( \mathcal{X}^*(k + 1) \) but \( A(\xi^{-1}) \) and \( B(\zeta^{-1}) \) are just the final results of computation which are not available in the instant when \( \mathcal{X}^*(k + 1) \) is needed. In order to enable the calculation, the values of parameters known from the preceding steps need to be used. Introducing

\begin{align*}
x^T(k) & = \left[ -x(k - 1), \ldots, -x(k - N), u(k - 1), \ldots, u(k - N) \right], \\
x(k) & = x^T(k) \mathcal{X}^*(k)
\end{align*}
or

\[(109)\quad x(k) = x^T(k) A(k-x),\]

where \(x\) is a small positive integer, we can overcome the mentioned difficulty.

For more details for this type of algorithm the reader is referred to D. Q. Mayne [1965] and to K. Y. Wong, E. Polak [1967]. Another procedure, called tally estimate, which may be included into the category of instrumental variable methods is that one published by V. Peterka, K. Šmuk [1969] and V. Peterka, A. Halousková [1970].

For the instrumental variable methods the parameter estimates will always converge to the true values. This is a well-known result effected by the properties of the off-line methods.

10. EXTENDED LEAST SQUARES METHOD

Consider a single input single output system given by

\[(110)\quad A(\xi^{-1}) y(k) = B(\xi^{-1}) u(k) + \frac{C(\xi^{-1})}{D(\xi^{-1})} e(k),\]

where

\[A(\xi^{-1}) = 1 + a_1 \xi^{-1} + \ldots + a_N \xi^{-N} \text{ etc.}\]

and

\[(111)\quad \xi^{-1} y(k) = y(k-1).\]

The publications P. C. Young [1971] and P. C. Young, R. Hastings-James [1970] are devoted to the general form (110). Most other authors consider the simplified form where either \(C(\xi^{-1}) = 1\) or \(D(\xi^{-1}) = 1\) (e.g. V. Panuska [1968]). In the following the case \(D(\xi^{-1}) = 1\) will be discussed. Moreover it is assumed that \(b_0 = 0\) and \(c_0 = 1\).

Introduce

\[(112)\quad \varphi^T(k) = [-y(k-1), \ldots, -y(k-N), u(k-1), \ldots, u(k-N),
\]

\[e(k-1), \ldots, e(k-N)],\]

\[(113)\quad \vartheta^T = [a_1, \ldots, a_N, b_1, \ldots, b_N, c_1, \ldots, c_N].\]

\(\vartheta^*\) corresponds to the estimate of the set of parameters in (113) and

\[(114)\quad \varphi^{*T}(k) = [-y(k-1), \ldots, -y(k-N), u(k-1), \ldots, u(k-N),
\]

\[e(k-1), \ldots, e(k-N)],\]

\[(115)\quad e(k) = y(k) - \vartheta^{*T}(k-1) \varphi^*(k).\]
The calculation of the error estimate $e(k)$ by means of past estimates of parameters in $A(k - 1)$ or, which is the same, by means of the relation

$$e(k) = y(k) - y^*(k(k - 1)),$$

is called extended least squares principle.

The respective recursive identification algorithm is given by

$$A(k) = A(k - 1) + M(k) e(k),$$

(116)

$$M(k) = \frac{P(k - 1) \phi^*(k)}{1 + \phi^*(k) P(k - 1) \phi^*(k)},$$

(117)

$$P(k) = P(k - 1) - \frac{P(k - 1) \phi^*(k) \phi^T(k) P(k - 1)}{1 + \phi^*(k) P(k - 1) \phi^*(k)} = [I - M(k) \phi^T(k)] P(k - 1),$$

(118)

L. Ljung and others [1975] have analyzed thoroughly the convergence properties of the formulas (116) through (118). For an exponentially stable system and for $\|e(k)\|^p < \infty$ for all $p > 0$, they concluded that if $A^*(k)$ tends to a stationary convergence point $A^*\opt$ with the probability strictly greater than zero, then

$$\delta^* e(k, A^*, A^*) = f(A^*) = 0$$

(119)

and all eigenvalues of $G^{-1}(A^*) H(A^*)$ have nonpositive real parts, where

$$G(A^*) = \delta^* \phi^*(k, A^*) \phi^T(k, A^*),$$

$$H(A^*) = \frac{d}{dA^*} f(A)|_{A^* = A^*},$$

$$f(A) = \delta^* \phi^*(k, A) e(k, A),$$

and provided that $G(A^*)$ is invertible and $\phi^*(k, A)$ and $e(k, A)$ are stationary processes.

In order to satisfy the above mentioned conditions, and in order to ensure the convergence of calculations, the modified recursive formulas were proposed

$$A^*(k) = A^*(k - 1) + M(k) e(k),$$

(120)

$$M(k) = \frac{P(k - 1) \phi^*(k)}{1 + \phi^*(k) P(k - 1) \phi^*(k)},$$

(121)

$$P(k) = [I - M(k) \phi^T(k)] P(k - 1),$$

(122)

$$e(k) = y(k) - A^*(k - 1) \phi(k),$$

(123)
where $x^*(k)$ is defined by

$$
(124) \quad C^{-1}_a(\xi^{(k)}) x^*(k) = \sigma^*(k)
$$

and $C^{-1}_a$ is given by the estimate $\mathcal{J}^*(k - 1)$. The algorithm (120) through (124) guarantees that the true value of $\mathcal{J}$ is always a possible convergence point.

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