P46

Pergamon

0005-1098(93)E0002-L

Automatica Vol. 30, No. 5, pp. 893–898, 1994

0005-1098/94 $7.00 + 0.00

Brief Paper

L_2-overbiased, L_2-underbiased and L_2-unbiased Estimation of Transfer Functions*

BART DE MOOR,†‡ MICHEL GEVERS§ and GRAHAM C. GOODWIN||

Key Words—Bias reduction; constraint theory; estimation theory; frequency response; identification; least-squares estimation; modeling; model reduction; parameter estimation.

Abstract—The identification of an undermodeled transfer function from input–output data is stated as a constrained optimization problem. The constraints determine the identification procedure, the residual error and whether on average the magnitude of the frequency response is L_2-overbiased, L_2-underbiased or L_2-unbiased, as measured by a certain weighted L_2-bias integral. The L_2-unbiased solutions are linear combinations of L_2-overbiased and L_2-underbiased solutions, which are precisely the classical least squares estimates. They can be obtained from the solution of certain eigenvalue problems.

1. *Introduction: identification as constrained minimization*

IN THIS PAPER, we put some identification approaches for undermodeling (i.e. the model set does not contain the "true" system) of SISO (single-input/single-output) systems into a general framework of constrained minimization. Using an L_2-error criterion, it will be shown that, depending on the constraints, the corresponding model can be L_2-overbiased, L_2-underbiased or L_2-unbiased, as quantified by a certain L_2-bias integral, which can be elegantly derived from the Lagrangean of the optimization problem. The main purpose of this work is to investigate the interaction between the specific constraints and some properties of the resulting identified model.

This paper is organized as follows: in the remainder of this section, we formulate the minimization problem that permits to identify linear models for SISO systems. In Section 2, we define an L_2-bias integral, which can be derived from the Lagrangean function of the optimization problem. In Section 3, we discuss the constraints that are allowed in our framework. It is shown how only linear, quadratic and multiplicative constraints lead to manageable algorithms (least squares or eigenvalue problems). In Section 4, we investigate the effects of linear constraints on the minimization problem (which will be least squares) and on the L_2-bias integral. In Section 5, we discuss quadratic constraints, which lead to eigenvalue problems, while Section 6 concentrates on multiplicative constraints. It is shown how the latter ones may result in L_2-unbiased models, which is the main result of this paper. Conclusions are formulated in Section 7.

Consider a true linear system $G_T(s)$ with input–output representation $y(t) = G_T(s)u(t)$. The model $G(s, \theta)$ is parametrized as:

$$G(s, \theta) = \frac{B(s, \theta)}{A(s, \theta)} = \frac{\beta_m s^m + \beta_{m-1} s^{m-1} + \cdots + \beta_1 s + \beta_0}{\alpha_n s^n + \alpha_{n-1} s^{n-1} + \cdots + \alpha_1 s + \alpha_0},$$

in which all coefficients are real. The parameter vector θ is defined as $\theta^t = (a^t b^t)$ with $a^t = (\alpha_0\, \alpha_1 \cdots \alpha_{n-1}\, \alpha_n)$ and $b^t = (\beta_0\, \beta_1 \cdots \beta_{m-1}\, \beta_m)$. We can rewrite the true system equation as:

$$y(t) = \frac{B(s, \theta)}{A(s, \theta)} u(t) + G_\Delta(s, \theta)u(t),$$

where $G_\Delta(s, \theta)$ represents the unmodelled dynamics. The input–output equation can also be written as:

$$A(s, \theta)y(t) - B(s, \theta)u(t) = A(s, \theta)G_\Delta(s, \theta)u(t). \quad (1)$$

Although the right-hand side could be considered as an equation error, equation (1) as such cannot be used for the purpose of identification because it contains transfer functions which are not proper, and hence require differentiation of signals. Therefore, we convert (1) into a system of proper transfer functions by introducing an observer polynomial $E(s)$ of degree $r \geq \max(m, n)$. Moreover, we can improve the signal-to-noise ratio and avoid aliasing effects by first filtering the data with a filter with transfer function $F(s)$. This filter can also be used to focus the model fit into some desired frequency range. Thus (1) becomes:

$$\frac{A(s)}{E(s)} F(s)y(t) - \frac{B(s)}{E(s)} F(s)u(t) = \frac{F(s)G_\Delta(s)A(s)}{E(s)} u(t) = e(t) \quad \text{(say)}, \quad (2)$$

* Received 4 June 1991; revised 11 February 1993; received in final form 5 June 1993. Preliminary versions of this paper were presented at the 9th IFAC/IFORS Symposium on Identification and System Parameter Estimation which was held in Budapest, Hungary during 8–12 July 1991. The Published Proceedings of this IFAC Meeting may be ordered from Elsevier Science Limited, The Boulevard, Langford Lane, Kidlington, Oxford OX5 1GB, U.K. This paper was recommended for publication in revised form by Associate Editor B. Wahlberg under the direction of Editor P. C. Parks. Corresponding author B. de Moor. Tel. +32 16 220931; Fax +32 16 221855; E-mail demoor@esat.kuleuven.ac.be.

† Dr De Moor is a research associate with the Belgian National Fund for Scientific Research. The results presented in this paper have been obtained within the framework of the Belgian Program on Concerted Research Actions and on the Interuniversity Attraction Poles initiated by the Belgian State, Prime Minister's Office, Science Policy Programming. The scientific responsibility rests with its authors.

‡ ESAT (Electronics, Systems, Automation, Technology), Katholieke Universiteit Leuven, Kardinaal Mercierlaan 94, B-3001 Leuven, Belgium.

§ Centre for Systems Engineering and Applied Mechanics, Université Catholique de Louvain, Bâtiment Euler, 4 Avenue Georges Lemaitre, B-1348 Louvain-la-Neuve, Belgium.

|| Centre for Industrial Control Science, Department of Electrical Engineering and Computer Science, University of Newcastle, NSW 2308, Australia.

where $e(t)$ is to be considered as an equation error.¶ It can be easily seen that the equation error is shaped by several factors, all of which could influence the result. We will however not concentrate on the precise selection of for instance the filters $E(s)$ and $F(s)$ in this paper, but refer to e.g. Ljung (1987) for more details on this matter.

We can rewrite equation (2) as

$$h'(t)\begin{pmatrix} a \\ b \end{pmatrix} = e(t)$$

in which each element of $h(t)$ is a filtered version of the input or output signals of the form:

$$\frac{F(s)s^i}{E(s)} y(t), \quad i = 0, \ldots, n$$

or

$$-\frac{F(s)s^j}{E(s)} u(t), \quad j = 0, \ldots, m.$$

The object function $J(\theta)$ is defined as

$$J(\theta) = \frac{1}{T}\int_0^T e^2(t)\,\mathrm{d}t$$
$$= \frac{1}{T}(a' b')\left[\int_0^T h(t)h'(t)\,\mathrm{d}t\right]\begin{pmatrix} a \\ b \end{pmatrix}. \quad (3)$$

Observe that this is a quadratic function of the components of a and b. The "information matrix" D is defined as:

$$D = \frac{1}{T}\int_0^T h(t)h'(t)\,\mathrm{d}t.$$

It is positive definite if $h(t)$ spans $\mathbb{R}^{m+n+2}$ over the interval $[0, T]$. This will be the case if the input $u(t)$ is "sufficiently rich" with respect to the dynamics of $G_T(s)$ over the interval $[0, T]$ and if $G_T(s)$ cannot be modelled by a rational transfer function with polynomial degrees less than m and n.

The problem of estimating the transfer function $G(s, \theta)$ can now be recast as a constrained minimization problem:

$$\min_{\text{over } \theta \in \mathbb{R}^{m+n+2}} J(\theta), \quad (4)$$

subject to constraints on $\theta = (a' b')$. Without constraints on a and b a trivial and useless solution to the minimization problem would be $a = 0$ and $b = 0$.

Using Parseval's Theorem, the time domain criterion (3) (with $T = \infty$) can be rewritten as the following frequency domain least squares criterion (see e.g. Ljung, 1987):

$$J(\theta) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} |L(j\omega)|^2 |A(j\omega, \theta)|^2 \times \left(\left|G_T(j\omega) - \frac{B(j\omega, \theta)}{A(j\omega, \theta)}\right|^2\right)\mathrm{d}\omega, \quad (5)$$

where

$$L(j\omega) = \frac{F(j\omega)}{E(j\omega)} U(j\omega).$$

The minimization of (4) or equivalently (5), subject to some specific constraints on a and b, yields a specific parameter vector $\hat{\theta}$ and a corresponding model $G(j\omega, \hat{\theta}) = B(j\omega, \hat{\theta})/A(j\omega, \hat{\theta})$. The fact that $\hat{\theta}$ can be described as the minimizing value of (5) shows how the fit between $G_T(j\omega)$ and the estimated model can be affected by specific choices of the filtered input spectrum $L(j\omega)$, i.e. how the L_2-bias can be shaped by appropriate frequency weighting.

¶ Observe that our derivation, especially the introduction of the observer polynomial, differs slightly from the standard procedure. Indeed, in for instance Salgado *et al.* (1990) α_n is *a priori* normalized to one. Then, (1) is rewritten as: $Ay - Bu + Ey - Ey = AG_\Delta u$ and then as $y = [(E - A)/E]y + [B/E]u + [AG_\Delta/E]u$ which is suited for a classical least squares identification algorithm. It is however the purpose of the present paper to study identification algorithms in general (not only least squares), hence the slightly more general derivation.

2. L_2-overbiased, L_2-underbiased and L_2-unbiased estimation

The constraints on a and b that are considered in this paper are of the form:

$$v(a, b) = 0, \quad (6)$$

where v is some linear or quadratic function of the coefficients in a and b. As we will show below, only linear and quadratic constraints lead to "manageable" numerical problems, namely least squares and eigenvalue problems.

Using a Lagrange multiplier λ, the Lagrangean for the optimization problem is given by

$$\mathscr{L}(a, b, \lambda) = J(a, b) - \lambda v(a, b).$$

In order to minimize (5) subject to (6) one has to solve the following set of $m + n + 3$ equations:

$$\frac{\partial \mathscr{L}}{\partial \alpha_i} = \frac{\partial J}{\partial \alpha_i} - \lambda\frac{\partial v}{\partial \alpha_i} = 0 \quad i = 0, \ldots, n, \quad (7)$$

$$\frac{\partial \mathscr{L}}{\partial \beta_j} = \frac{\partial J}{\partial \beta_j} - \lambda\frac{\partial v}{\partial \beta_j} = 0 \quad j = 0, \ldots, m \quad (8)$$

$$v(a, b) = 0. \quad (9)$$

It is straightforward to derive from (5) that (we omit $j\omega$ for clarity where possible):

$$\frac{\partial J}{\partial \alpha_i} = \frac{1}{2\pi}\int_{-\infty}^{+\infty} |L|^2 [(j\omega)^i A^* G_T G_T^* + (-j\omega)^i A G_T G_T^* - (j\omega)^i G_T B^* - (-j\omega)^i B G_T^*]\,\mathrm{d}\omega$$

$$\frac{\partial J}{\partial \beta_i} = \frac{1}{2\pi}\int_{-\infty}^{\infty} |L|^2 [(j\omega)^i B^* + (-j\omega)^i B - (-j\omega)^i A G_T - (j\omega)^i G_T^* A^*]\,\mathrm{d}\omega.$$

From this we find:

$$\sum_{i=0}^{n} \alpha_i \frac{\partial J}{\partial \alpha_i} - \sum_{i=0}^{m} \beta_i \frac{\partial J}{\partial \beta_i} = \frac{2}{2\pi}\int_{-\infty}^{\infty} |L|^2 |A|^2 \times \left(|G_T|^2 - \frac{|B|^2}{|A|^2}\right)\mathrm{d}\omega = 2V(\theta) \quad \text{(say)}. \quad (10)$$

The parameter function $V(\theta)$ will be called the L_2-bias integral. The value of (10), for a specific model $\hat{\theta}$, reflects the bias, in a weighted square sense, between the magnitude of the true transfer function and that of the estimated model transfer function. Note that the frequency weighting is the same in (10) as in the identification criterion (5). Loosely speaking, the difference between (5) and (10) is that (5) is the weighted sum of differences squared, while (10) is the weighted sum of squared differences.

We shall call the estimated model L_2-overbiased if $V(\hat{\theta}) < 0$. In this case, the magnitude of the model's transfer function as a function of frequency, is on the average larger than the one of the true system. We call the model L_2-underbiased if $V(\hat{\theta}) > 0$. On the average, the magnitude of the model's transfer function is smaller than the one of the true system. The model is L_2-unbiased if $V(\hat{\theta}) = 0$. Intervals where the magnitude of the model's transfer function dominates the one of the true model, are "compensated" by regions where the true system's magnitude is larger than that of the model.

We can now combine equations (7)–(9) and equation (10) to find that:

$$2V(\theta) = \lambda\left(\sum_{i=0}^{n} \alpha_i \frac{\partial v(a, b)}{\partial \alpha_i} - \sum_{j=0}^{m} \beta_j \frac{\partial v(a, b)}{\partial \beta_j}\right). \quad (11)$$

The interpretation is the following: While we minimize the residual mean square error (5) subject to the constraint (6), we can at the same time obtain the numerical value of the L_2-bias integral (10) by substituting the optimal value of the Lagrange multiplier λ and the optimal parameter values in (11).

In Salgado *et al.* (1990), it was observed that for a parametrization of the model transfer function $G(s)$ with $\alpha_n = 1$, the resulting least squares solution provides an underbiased model. In Gevers (1990), it was observed that the constraint $\beta_m = 1$ results in an overbiased model. These observations and the conjecture formulated in Gevers (1990) have stimulated the present research, in particular the quest for an unbiased identification scheme.

The main result of this paper is the observation that the specific choice for a constraint on the vectors a and b determines the identification method on the one hand (least squares, eigenvalue decomposition, etc.), the residual mean square error (3) and the bias integral (10) on the other hand.

It will be shown how, by a careful choice of the constraints, one may construct identification schemes that are unbiased, and at the same time minimize $J(\hat{\theta})$ among all unbiased models.

Throughout we shall use the following notation: the information matrix D is partitioned as

$$D = \begin{array}{c} \\ n+1 \\ m+1 \end{array} \begin{array}{c} \begin{array}{cc} n+1 & m+1 \end{array} \\ \begin{pmatrix} D_{aa} & D_{ab} \\ D'_{ab} & D_{bb} \end{pmatrix} \end{array}.$$

The inverse of D is partitioned as:

$$D^{-1} = \begin{array}{c} \\ n+1 \\ m+1 \end{array} \begin{array}{c} \begin{array}{cc} n+1 & m+1 \end{array} \\ \begin{pmatrix} P & Q \\ Q' & R \end{pmatrix} \end{array},$$

where $P = (D_{aa} - D_{ab}D_{bb}^{-1}D'_{ab})^{-1}$, $Q = -D_{aa}^{-1}D_{ab}(D_{bb} - D'_{ab}D_{aa}^{-1}D_{ab})^{-1}$ and $R = (D_{bb} - D'_{ab}D_{aa}^{-1}D_{ab})^{-1}$. It is also a positive definite matrix and both P and R are square, symmetric, positive definite matrices.

For reasons explained in De Moor and Vandewalle (1986, 1990), the kth column of D^{-1} will be referred to as the kth least squares solution.

Estimates are denoted by a superscript "^". The notation $\mathbf{1}_k$ refers to the unit vector, which is zero everywhere, except for its kth component, which is one.

3. *What constraints are allowed?*

Before considering in detail some possible constraints for the optimization problem (4), let us first determine what type of constraints are allowed. The model class in which we are interested is completely specified by the degrees of the numerator and denominator of the transfer function $G(s, \theta)$. Constraints on the coefficients of both numerator and denominator must not further restrict this model class. For instance, two constraints of the form $a'a = 1 = b'b$ are not allowed since generically a transfer function with numerator degree m and denominator degree n will not satisfy these constraints simultaneously. In general, we can only allow constraints that leave the ratio of the polynomials $A(s, \theta)$ and $B(s, \theta)$ unmodified for all values of s. This requirement is satisfied by the following constraints:

Linear constraints: a linear constraint of the form $\alpha_k = 1$ for any k with $0 \le k \le n$ will be discussed in Section 4. A constraint of the form $\beta_k = 1$ for $0 \le k \le m$ leads to completely similar conclusions.

Quadratic constraints: quadratic constraints of the form $a'a = 1$ or $b'b = 1$ are treated in Section 5, together with a quadratic constraint of the form $a'a + b'b = 1$.

Multiplicative constraints: constraints of the form $\alpha_k\beta_l = \pm 1$ are investigated in Section 6, where we also treat constraints of the form $\sum_{k=1}^{r} \alpha_k\beta_k = \pm 1$ with $r \le m$.

Observe that for the last case, the "$\pm$" refers to the fact that we are not allowed to impose *a priori* the sign of the (sums of) product(s) since this would imply a restriction of the model class. For instance, a constraint of the form $\alpha_0\beta_0 = 1$ would imply that the static gain, which is β_0/α_0, is positive. This constraint is obviously restricting the model class. For a given transfer function $G(s) = B(s)/A(s)$, one can always find a real scalar ρ such that $G(s) = (\rho B(s))/(\rho A(s))$ and the coefficients of the polynomials $\rho A(s)$ and $\rho B(s)$ satisfy any of the mentioned constraints. While from the theoretical point of view all these models are equivalent, their application in the minimization problem (4) will yield different results.

4. *Linear constraints*

Consider the minimization of (4) with a linear constraint on the kth component of a:

$$\alpha_{k-1} = 1, \tag{12}$$

where k is a fixed, user-defined index (but the user can of course pick out any index she would desire). We then find from (7)–(9) that:

$$D\begin{pmatrix} a \\ b \end{pmatrix} = \mathbf{1}_k\lambda/2.$$

Hence

$$\begin{pmatrix} \hat{a} \\ \hat{b} \end{pmatrix} = D^{-1}\mathbf{1}_k\lambda/2,$$

which implies that the solution vector $(\hat{a}'\,\hat{b}')'$ is proportional to the kth column of D^{-1}. The Lagrange multiplier λ can be determined from the constraint $\alpha_{k-1} = 1$:

$$J(\hat{\theta}) = \lambda/2 = 1/p_{kk} > 0.$$

For the L_2-bias (10) we find from (11):

$$V(\hat{\theta}) = \lambda/2.$$

Hence, the bias integral is precisely equal to the kth least squares residual! Its positivity implies that the linear constraint (12) leads to an L_2-underbiased model [which was observed in Salgado *et al.* (1990) for the constraint $\alpha_n = 1$].

Similarly, it can be derived from (7)–(9) and (11) that a constraint of the form:

$$\beta_{k-1} = 1, \tag{13}$$

where again, k is a fixed index, leads to an L_2-overbiased model:

$$V(\hat{\theta}) = -J(\hat{\theta}) = -\frac{1}{r_{kk}} < 0.$$

This was observed in Gevers (1990) for the constraint $\beta_m = 1$. Here we find the more general result that the overbiasedness holds for all constraints (13). The solution vector $(a'\,b')$ is now proportional to the $(k+n+1)$th column of D^{-1} and the Lagrange multiplier follows from the constraint (13).

Because all the solutions from the linearly constrained optimization problems of this section can be obtained via a "classical" linear least squares scheme (see e.g. De Moor and Vandewalle, 1986, 1988, 1990; Swevers *et al.*, 1991), we propose to call the columns of D^{-1} (normalized such that the constrained component is one), the *linear least squares solutions.* Hence there are $m + n + 2$ linear least squares solutions, corresponding to the $m + n + 2$ possible constraints (12) and (13).

5. *Quadratic constraints*

With a quadratic constraint of the form:

$$a'a = 1, \tag{14}$$

we find from (7)–(9) that

$$D_{aa}a + D_{ab}b = a\lambda, \tag{15}$$

$$D'_{ab}a + D_{bb}b = 0. \tag{16}$$

Since D is invertible and positive definite, it follows from Cauchy's eigenvalue interlacing property (Golub and Van Loan, 1989, p. 411) that the submatrix D_{bb} is also invertible. Hence $b = -D_{bb}^{-1}D'_{ab}a$, so that

$$(D_{aa} - D_{ab}D_{bb}^{-1}D'_{ab})a = a\lambda, \quad a'a = 1.$$

Hence, we need to solve the eigenvalue problem for the Schur complement of the matrix D_{bb} in D (which is symmetric and positive definite) for its minimal eigenvalue and corresponding eigenvector. Observe that:

$$\begin{pmatrix} \hat{a} \\ \hat{b} \end{pmatrix} = \begin{pmatrix} P \\ Q' \end{pmatrix}\hat{a}\lambda.$$

Hence in this case the solution is a linear combination of the first $n+1$ columns of D^{-1}, which are the $n+1$ least squares solutions of our identification problem, corresponding to the $n+1$ possible constraints $\alpha_0 = 1, \ldots, \alpha_n = 1$.

We also observe from (15) and (16) that the optimal value $J(\hat{\theta})$ is given by:

$$J(\hat{\theta}) = (\hat{a}'\,\hat{b}')D\begin{pmatrix}\hat{a}\\ \hat{b}\end{pmatrix} = \lambda.$$

Using (10) together with (15) and (16) we find:

$$V(\hat{\theta}) = J(\hat{\theta}) = \lambda > 0.$$

The last two expressions show that this identification scheme, which gives as a result a linear combination of L_2-underbiased models, is itself L_2-underbiased.

Similarly, for the constraint

$$b'b = 1, \tag{17}$$

the solution vector b is the eigenvector of the Schur complement of D_{aa} in D, corresponding to the smallest eigenvalue λ that satisfies:

$$(D_{bb} - D'_{ab}D_{aa}^{-1}D_{ab})b = b\lambda, \quad b'b = 1. \tag{18}$$

The residual mean square error (3) is equal to the smallest eigenvalue λ of $D_{bb} - D'_{ab}D_{aa}^{-1}D_{ab}$ (which is a positive definite matrix). The solution in this case is a linear combination of the last $m+1$ columns of D^{-1}, which are the $m+1$ least squares solution of our identification problem, corresponding to the $m+1$ possible constraints $\beta_0 = 1, \ldots, \beta_m = 1$. The value of the bias integral (10) is given by $-\lambda$ and is always negative. Hence, we have a systematic overestimation of the magnitude: the identified model is L_2-overbiased.

Observe that the identification method which follows from $b'b = 1$ [i.e. the eigenvalue problem (18)] might be advantageous from the computational point of view if the numerator degree m is small.

Obviously, the constraint (14) can be viewed as a special case of constraints of the form:

$$\sum_{i=0}^{r_1} \alpha_i^2 = 1, \tag{19}$$

with $r_1 \le n$. This constraint will lead to an $(r_1+1)\times(r_1+1)$ symmetric positive definite eigenvalue problem. The solution will be a linear combination of the first r_1+1 columns of D^{-1}, which are the least squares solutions corresponding to $\alpha_0 = 1, \ldots, \alpha_{r_1} = 1$. The L_2-bias integral will be negative and hence we have an L_2-underbiased identification scheme. It is interesting to note that, while all identifications with (19) are L_2-underbiased, the minimum of the residual mean square error (3) decreases for increasing values of r_1. This is a direct consequence of the eigenvalue interlacing theorem applied to the upper $(r_1+1)\times(r_1+1)$ blocks of the matrix D^{-1} for $r_1 = 0, \ldots, n$.

Similar conclusions hold of course for constraints on b of the type $\sum_{j=0}^{r_2} \beta_j^2 = 1$ with $r_2 \le m$. In this case, we have always an L_2-overbiased identification.

We can also combine the quadratic constraints (14) and (17) into one constraint as

$$a'a + b'b = 1. \tag{20}$$

It now follows from (7)–(9) that:

$$D\begin{pmatrix}a\\ b\end{pmatrix} = \begin{pmatrix}a\\ b\end{pmatrix}\lambda.$$

Obviously, the optimum value of λ is precisely the smallest eigenvalue $\lambda_{\min}$ of the matrix D. The solution for the vectors of polynomial coefficients a and b is given by:

$$\begin{pmatrix}\hat{a}\\ \hat{b}\end{pmatrix} = v_{\min},$$

where $v_{\min}$ is the eigenvector of D corresponding to the smallest eigenvalue, normalized such that its norm equals one. From (11) we find that:

$$V(\hat{\theta}) = \lambda_{\min}(\hat{a}'\hat{a} - \hat{b}'\hat{b}).$$

Hence, the value of the L_2-bias integral depends not only on the smallest eigenvalue of D, but also on the difference of the norms of the vectors of polynomial coefficients [which are constrained by (20)]. This identification scheme is L_2-underbiased if $\hat{a}'\hat{a} - \hat{b}'\hat{b} > 0$ and L_2-overbiased if $\hat{a}'\hat{a} - \hat{b}'\hat{b} < 0$.

The constraints (14), (17), (19) and (20) may all be considered as a special case of a constraint of the form:

$$\sum_{i=0}^{r_1} \alpha_i^2 + \sum_{j=0}^{r_2} \beta_j^2 = 1, \tag{21}$$

with $0 \le r_1 \le n$ and $0 \le r_2 \le m$. This type of constraint leads to an $(r_1+r_2+2)\times(r_1+r_2+2)$ eigenvalue problem for a symmetric submatrix of D (which is necessarily positive definite because of the eigenvalue interlacing property). However, also because of the eigenvalue interlacing property, we know that only with the full quadratic constraint (20) (i.e. for $r_1 = n$ and $r_2 = m$), we get the minimal possible eigenvalue over all quadratic constraints, which is the minimal eigenvalue of D.

As an example, consider the constraint

$$\alpha_0^2 + \beta_0^2 = 1, \tag{22}$$

we find

$$D\begin{pmatrix}\alpha_0\\ a_2\\ \beta_0\\ b_2\end{pmatrix} = \begin{pmatrix}\alpha_0\\ 0\\ \beta_0\\ 0\end{pmatrix}\lambda,$$

where a_2 and b_2 contain the components of a and b except for the first one. Observe that

$$\begin{pmatrix}\alpha_0\\ a_2\\ \beta_0\\ b_2\end{pmatrix} = D^{-1}\begin{pmatrix}\alpha_0\\ 0\\ \beta_0\\ 0\end{pmatrix}\lambda, \tag{23}$$

which demonstrates that the solution vector is a linear combination of the first and the $(n+2)$th column of D^{-1}, which are two least squares solutions, corresponding to the constraints $\alpha_0 = 1$ and $\beta_0 = 1$. The coefficients α_0 and β_0 can be determined from the 2×2 symmetric positive definite eigenvalue problem:

$$\begin{pmatrix}p_{11} & q_{11}\\ q_{11} & r_{11}\end{pmatrix}\begin{pmatrix}\alpha_0\\ \beta_0\end{pmatrix} = \begin{pmatrix}\alpha_0\\ \beta_0\end{pmatrix}\kappa, \tag{24}$$

where $\kappa = 1/\lambda$ and p_{11}, q_{11} and r_{11} are the leading elements of P, Q, R. Obviously, we must take the solution corresponding to the maximal eigenvalue κ, the inverse of which will be the minimum of the residual mean square error $J(\theta)$ (3). The coefficients of a_2 and b_2 follow from (23). It is also easy to find that the value of the bias integral $V(\theta)$ (10) is given by $\lambda(\alpha_0^2 - \beta_0^2)$. Depending on its sign, the identification will be L_2-over- or L_2-underbiased.

As another example, consider the constraint:

$$\alpha_0^2 + \alpha_1^2 + \beta_0^2 + \beta_1^2 = 1.$$

We now need to find the maximal eigenvalue κ of the 4×4 symmetric positive definite eigenvalue problem:

$$\begin{pmatrix}p_{11} & p_{12} & q_{11} & q_{12}\\ p_{12} & p_{22} & q_{21} & q_{22}\\ q_{11} & q_{21} & r_{11} & r_{12}\\ q_{12} & q_{22} & r_{12} & r_{22}\end{pmatrix}\begin{pmatrix}\alpha_0\\ \alpha_1\\ \beta_0\\ \beta_1\end{pmatrix} = \begin{pmatrix}\alpha_0\\ \alpha_1\\ \beta_0\\ \beta_1\end{pmatrix}\kappa. \tag{25}$$

The minimum value of the residual mean square error (3) will then be given by $1/\kappa$. It is a direct consequence of the eigenvalue interlacing theorem that the maximal eigenvalue of (25) will be larger than the maximal eigenvalue of (24). Hence, the corresponding residual mean square error $J(\theta)$ (3) will be smaller! So the prize to be paid for a smaller residual is the solution of a larger eigenvalue problem.

We can however not control the L_2-(un)biasedness *a priori* as this depends on the sign of $\lambda(\alpha_0^2+\alpha_1^2-\beta_0^2-\beta_1^2)$, which can only be determined *a posteriori*.

One might even consider constraints that are asymmetric in the number of components of a and b, for instance: $\alpha_0^2+\alpha_1^2+\beta_0^2=1$. Now, we need to solve a 3×3 symmetric positive definite eigenvalue problem.

We may conclude that with this type of quadratic constraints, one can decrease the norm of the residual by solving increasingly larger eigenvalue problems. The resulting sign of the L_2-bias integral however can not be predicted *a priori*.

6. *Multiplicative constraints*

All identification schemes so far minimize the residual mean mean square error (3) but are L_2-biased with respect to the frequency criterion (10). The question remains whether there are certain types of constraints that give an L_2-unbiased model. Consider the minimization problem (4) with a constraint of the form:

$$\alpha_{k-1}\beta_{l-1}=\gamma, \tag{26}$$

where k and l are fixed indices and γ is a given real number.

We will show that this type of constraints leads to L_2-unbiased models. First observe that we are not free in the choice of the sign of γ. Indeed, assume that $k=l=1$, then the real number β_0/α_0 is the static gain of the transfer function. Therefore, fixing the sign of γ corresponds to fixing the sign of the static gain, which implies a restriction on the model class. However, for the moment, we shall assume that we know the sign of γ. It will be shown below that we really do not need this information *a priori*. As a matter of fact, the identification scheme will always automatically allow both choices.

From (7)–(9) we find:

$$D_{aa}a+D_{ab}b=\mathbf{1}_k\beta_{l-1}\lambda/2, \tag{27}$$

$$D'_{ab}a+D_{bb}b=\mathbf{1}_l\alpha_{k-1}\lambda/2. \tag{28}$$

It follows from the invertibility of D that:

$$\begin{pmatrix}\hat a\\ \hat b\end{pmatrix}=D^{-1}\begin{pmatrix}\mathbf{1}_k\beta_{l-1}\\ \mathbf{1}_l\alpha_{k-1}\end{pmatrix}\lambda/2. \tag{29}$$

From this equation, we see that the optimal $\hat\theta$ can be obtained as a linear combination of two columns of D^{-1}, which are precisely two least squares solutions! The coefficients α_{k-1} and β_{l-1} can be calculated from the 2×2 eigenvalue problem:

$$\begin{pmatrix}q_{kl} & p_{kk}\\ r_{ll} & q_{lk}\end{pmatrix}\begin{pmatrix}\alpha_{k-1}\\ \beta_{l-1}\end{pmatrix}=\begin{pmatrix}\alpha_{k-1}\\ \beta_{l-1}\end{pmatrix}\kappa, \tag{30}$$

where $\kappa=2/\lambda$. The eigenvalues are given by:

$$\kappa=q_{kl}\pm\sqrt{r_{ll}p_{kk}} \tag{31}$$

and are always real since the diagonal elements of P and R are positive. The 2×2 matrix in (30) is obtained by interchanging the columns of the 2×2 matrix:

$$\begin{pmatrix}p_{kk} & q_{kl}\\ q_{lk} & r_{ll}\end{pmatrix}. \tag{32}$$

But the 2×2 matrix in (32) is positive definite as a consequence of the eigenvalue interlacing property. In particular this implies that $p_{kk}>0$, $r_{ll}>0$, $p_{kk}r_{ll}>q_{kl}q_{lk}$. Hence there is always a positive and a negative eigenvalue in (31). Recall that we could not *a priori* fix the sign of γ in $\alpha_{k-1}\beta_{l-1}=\gamma$. But here we find precisely that such an *a priori* preference is not needed because we will always have the choice between a positive and a negative eigenvalue. In particular, when $k=1$ and $l=1$, the product $\alpha_0\beta_0$ is either positive or negative, corresponding to a static gain β_0/α_0 which is either positive or negative. We are interested in the eigenvalue κ with the largest absolute value (which corresponds to the λ with the least absolute value). Its sign will also determine the sign of γ. The eigenvectors have to be normalized such that $|\alpha_{k-1}\beta_{l-1}|=|\gamma|$. Having determined the coefficients α_{k-1}, β_{l-1} and λ, the remaining coefficients are determined from (29).

Premultiplying (27) with $\hat a'$ and (28) with $\hat b'$ and adding, we find:

$$J(\hat\theta)=(\hat a'\ \hat b')D\begin{pmatrix}\hat a\\ \hat b\end{pmatrix}=\hat\alpha_{k-1}\hat\beta_{l-1}\lambda=\gamma\lambda.$$

Obviously, from $J(\hat\theta)>0$, we have that if $\gamma>0$, then $\lambda>0$ and if $\gamma<0$, we must have $\lambda<0$. For any specific choice of γ, we want to minimize $J(\theta)$, hence it suffices to look for the value of λ with least absolute value. From (10), it follows that

$$2V(\hat\theta)=(\hat a'\mathbf{1}_k\hat\beta_{l-1}-\hat b'\mathbf{1}_l\hat\alpha_{k-1})\lambda/2=0.$$

Hence, this identification scheme is L_2-unbiased!

The results just derived have a very appealing interpretation: recall that the columns of D^{-1} are precisely the least squares solutions. The first $n+1$ columns of D^{-1} are the solutions to the optimization problems (4) with one linear constraint (12) on a coefficient of $A(s)$, while the remaining $m+1$ columns are the solutions for a linear constraint (13) on a coefficient of $B(s)$. The former ones yield L_2-underbiased models while the latter ones yield L_2-overbiased models. For the constraint (26), we now see from (29) that the solution is described as a linear combination of the two least squares solutions obtained with a linear constraint on α_{k-1} and one on β_{l-1}. The respective weights attached to these two solutions follow from the 2×2 eigenvalue problem (30). The resulting solution is L_2-unbiased. Hence, we find that a certain linear combination of an L_2-overbiased and an L_2-underbiased solution, results in an L_2-unbiased one!

The multiplicative constraint (26) can be generalized to a constraint of the form:

$$\sum_{i=1}^{r}\alpha_{i-1}\beta_{i-1}=\gamma\quad 1\le r\le m+1, \tag{33}$$

where r is fixed and $\gamma\in\mathbb{R}$ is given. For the same reason as before, the sign of γ is not fixed but will be determined furtheron. For the time being however, it is assumed that γ is a fixed given real number. Using the notation $a_r=(\alpha_0\cdots\alpha_{r-1})'$ and $b_r=(\beta_0\cdots\beta_{r-1})'$ we find from (7)–(9) that:

$$D\begin{pmatrix}a\\ b\end{pmatrix}=\begin{pmatrix}b_r\\ 0\\ a_r\\ 0\end{pmatrix}\lambda/2.$$

Observe that if $\hat\theta$ is a solution, then

$$J(\hat\theta)=(\hat a'\ \hat b')D\begin{pmatrix}\hat a\\ \hat b\end{pmatrix}=\gamma\lambda.$$

Since $J(\hat\theta)$ is always positive, it follows that λ and γ must have the same sign. We need to find the least absolute value of λ. It also follows from (10) that:

$$V(\hat\theta)=0$$

Hence, the resulting identification scheme is L_2-unbiased! From the nonsingularity of D, it follows that:

$$\begin{pmatrix}a\\ b\end{pmatrix}=\begin{pmatrix}P & Q\\ Q' & R\end{pmatrix}\begin{pmatrix}b_r\\ 0\\ a_r\\ 0\end{pmatrix}\lambda/2. \tag{34}$$

From this equation we see that the solution will be a linear combination of the first $r+1$ columns of D^{-1} and its columns $(n+2)$ up to $(n+r+2)$. The coefficients $\alpha_i, \beta_i, i=0,\ldots,r-1$ can be determined from the $2r\times 2r$ eigenvalue problem:

$$\begin{pmatrix}Q_r & P_r\\ R_r & Q'_r\end{pmatrix}\begin{pmatrix}a_r\\ b_r\end{pmatrix}=\begin{pmatrix}a_r\\ b_r\end{pmatrix}\kappa, \tag{35}$$

TABLE 1. THIS TABLE SUMMARIZES THE MAIN RESULTS. LINEAR CONSTRAINTS LEAD TO LEAST SQUARES PROBLEMS AND SOLUTIONS THAT ARE L_2 UNDER- OR OVERBIASED. QUADRATIC CONSTRAINTS LEAD TO EIGENVALUE PROBLEMS AND ARE L_2 UNDER- OR OVERBIASED. MULTIPLICATIVE CONSTRAINTS GIVE L_2 UNBIASED RESULTS.

Constraint	Linear relation	Residual error $J(\hat{\theta})$	Bias $V(\hat{\theta})$
$\alpha_k = 1$	kth least squares solutions	kth least squares residual	Underbiased
$\beta_k = 1$	$(k+n+1)$th least squares solution	$(k+n+1)$th least squares residual	Overbiased
$a'a = 1$	Eigenvector of Schur complement	Smallest eigenvalue of Schur complement	Underbiased
$b'b = 1$			Overbiased
$a'a + b'b = 1$	Eigenvector of D	Smallest eigenvalue of D	Overbiased $(a'a - b'b < 0)$ Underbiased $(a'a - b'b > 0)$
$\alpha_{k-1}\beta_{l-1} = \gamma$	Linear combination of two least squares solutions	Eigenvalue of 2×2 matrix	Unbiased
$\sum_{i=1}^{r} \alpha_{i-1}\beta_{i-1} = \gamma$	Linear combination of $2r$ least squares solutions	Eigenvalue of $2r \times 2r$ matrix	Unbiased

where $\kappa = 2/\lambda$. Here P_r, Q_r and R_r are the $r \times r$ leading submatrices of P, Q and R respectively. The matrix in (35) is obtained by interchanging the relevant block columns of the partitioned matrix D^{-1}. We are interested in the real eigenvalue κ of maximal absolute value. The corresponding eigenvector should be normalized so as to satisfy (33). The other coefficients can be determined from (34). It is interesting to note that all eigenvalues of (35) are real and that there are r positive and r negative ones. This is a direct consequence of the following lemma:

Lemma 1. Let T be a $2q \times 2q$ real, symmetric, positive definite matrix with square $q \times q$ blocks: $T = \begin{pmatrix} T_{11} & T_{12} \\ T'_{12} & T_{22} \end{pmatrix}$. Then the eigenvalues of the matrix $\begin{pmatrix} T_{12} & T_{11} \\ T_{22} & T'_{12} \end{pmatrix}$ are real, q of them are positive and q negative.

Proof. Define the block permutation matrix $\bar{I}$ as $\bar{I} = \begin{pmatrix} 0 & I_q \\ I_q & 0 \end{pmatrix}$. We are interested in the eigenvalues λ of $T\bar{I}$, which are the roots of the characteristic equation $\det(T\bar{I} - \lambda I_{2q}) = 0$. Let the eigenvalue decomposition of T be $T = X\Lambda X'$. Then:

$$\begin{aligned} \det(\bar{I} - \lambda T^{-1}) = 0 &\Leftrightarrow \det(\bar{I} - \lambda X\Lambda^{-1}X') = 0 \\ &\Leftrightarrow \det(X\Lambda^{-1/2}[\Lambda^{1/2}X'\bar{I}X\Lambda^{1/2} \\ &\quad - \lambda I_{2q}]\Lambda^{-1/2}X') = 0 \\ &\Leftrightarrow \det(\Lambda^{1/2}X'\bar{I}X\Lambda^{1/2} - \lambda I_{2q}) = 0. \end{aligned}$$

So the eigenvalues of $T\bar{I}$ are the eigenvalues of $\Lambda^{1/2}X'\bar{I}X\Lambda^{1/2}$, which is symmetric, hence has real eigenvalues. Furthermore, $\Lambda^{1/2}X'\bar{I}X\Lambda^{1/2}$ is congruent to $\bar{I}$, the eigenvalues of which are $+1$ (q times) and -1 (q times). Sylvester's Theorem (Golub and Van Loan, 1989, p. 416) states that a congruence transformation preserves the inertia, which completes the proof. □

7. *Conclusions*

In this paper, we have shown how the estimation of undermodelled dynamics can be formulated as a constrained optimization technique. The constraints determine the identification method to be used (solving sets of linear equations or eigenvalue problems), the value of the residual mean square error and whether the magnitude of the estimated transfer function is L_2-overbiased, L_2-underbiased as measured by a frequency weighted L_2-bias-integral. A survey of the results is given in Table 1. "Square root" versions of the algorithms in this paper are derived in Swevers *et al.* (1991). These are algorithms where the explicit formation of the matrix D is avoided and the data matrix itself is used. The least squares solutions are obtained from QR-decompositions of the data matrix while the eigenvalue decompositions are replaced by singular value decompositions. In Swevers *et al.* (1991) we show that these square root versions are much more robust in certain modelling situations.

References

De Moor, B. and J. Vandewalle (1986). A geometrical approach to the maximal corank problem in the analysis of linear relations. *Proc. of the 25th IEEE Conference on Decision and Control*, pp. 1990–1996. Athens, Greece.

De Moor, B. and J. Vandewalle (1988). The uncertainty principle of mathematical modeling. *IFAC Symposium on Identification and System Parameter Estimation*, pp. 2017–2021. Beijing, P.R. China.

De Moor, B. and J. Vandewalle (1990). A unifying theorem for linear and total linear least squares identification schemes. *IEEE Transactions on Automatic Control*, **35**, 563–566.

Gevers, M. (1990). Estimation of transfer functions: underbiased or overbiased. *Proc. 29th Conference on Decision and Control*, pp. 3200–3201. Honolulu, Hawaii.

Golub, G. H. and C. F. Van Loan (1989). *Matrix Computations*, 2nd ed. Johns Hopkins University Press, Baltimore, MD.

Ljung, L. (1987). *System Identification: Theory for the User.* Prentice-Hall, Englewood Cliffs, NJ.

Salgado, M. E., C. E. De Souza and G. C. Goodwin (1990). Qualitative aspects of the distribution of errors in least squares estimation. *Automatica*, 97–101.

Swevers, J., B. De Moor and H. Van Brussel (1991). Square-root algorithms for overbiased, underbiased or unbiased transfer function estimation. ESAT-SISTA Report February 1991, Department of Electrical Engineering, Katholieke Universiteit Leuven, Belgium.