Optimally Conditioned Instrumental Variable Approach for Frequency-Domain System Identification

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Abstract

Accurate frequency-domain system identification demands for reliable computational algorithms. The aim of this paper is to develop a new algorithm for parametric system identification with favorable convergence properties and optimal numerical conditioning. Recent results in frequency-domain instrumental variable identification are exploited, which lead to enhanced convergence properties compared to classical identification algorithms. In addition, bi-orthonormal polynomials with respect to a data-dependent bi-linear form are introduced for system identification. Hereby, optimal numerical conditioning of the relevant system of equations is achieved. This is shown to be particularly important for the class of instrumental variable algorithms, for which numerical conditioning is typically quadratic compared to alternative frequency-domain identification algorithms. Superiority of the proposed algorithm is demonstrated by means of both simulation and experimental results.

Keywords: System identification; Identification algorithms; Numerical methods; Matrix inversion; Condition numbers

1. Introduction

Frequency-domain system identification (Pintelon & Schoukens, 2001), (McKelvey, 2002) is of significant importance for a broad class of applications, since it enables i) straightforward data reduction, ii) straightforward combination of multiple data sets, iii) direct estimation and use of nonparametric noise models, and iv) a direct connection to control-relevant identification criteria.

Many parametric identification techniques based on frequency-domain data involve a nonlinear least-squares problem. Here, the nonlinearity arises from the parametrization of the poles in the denominator polynomial. In Levy (1959), the nonlinear problem is approximated using a single linear least-squares problem. However, this introduces an *a priori* unknown weighting function. The SK-algorithm (Sanathanan & Koerner, 1963) mitigates the effect of such weighting through iterations. In Bayard (1994), De Callafon et al. (1996), the SK-algorithm is generalized to multivariable systems. Nevertheless, two aspects require further attention.

On the one hand, frequency-domain identification problems are typically numerically ill-conditioned. Several partial solutions exist, including i) frequency scaling (Pintelon & Kollár, 2005), ii) amplitude scaling (Hakvoort & Van den Hof, 1994), and iii) the use of orthonormal polynomials and orthonormal rational functions with respect to a continuous inner product, see, e.g., Heuberger et al. (2005) and Ninness & Hjalmarsson (2001) for a connection with numerical properties. These approaches confirm that ill-conditioning is an important aspect in system identification applications and they typically improve numerical conditioning. However, these partial solutions may be insufficient to reliably solve complex frequency-domain identification problems. Therefore, in Van Herpen et al. (2012b) and Oomen & Steinbuch (to appear), an approach is presented that leads to optimal numerical conditioning of the SK-algorithm by using polynomials that are orthonormal with respect to a data-based discrete inner product, see Reichel et al. (1991) and Van Barel & Bultheel (1995) for a definition and earlier results.

On the other hand, the fixed point of the SK-algorithm generally does not correspond to a (local) minimum of the nonlinear least-squares criterion, as shown in Whitfield (1987). Consequently, the SK-algorithm is typically used as an initialization for subsequent Gauss-Newton iterations, see, e.g., Bayard (1994) and Pintelon & Schoukens (2001, Sect. 7.9.1), which guarantees convergence to a (local) minimum.

Recently, in Douma (2006, Sect. 3.5.3 and 3.5.8), an alternative frequency-domain identification algorithm has been formulated, in which a fixed point of the iterations corresponds to an optimum of the objective function. This renders a Gauss-Newton iteration superfluous, potentially enabling an increase of algorithm efficiency. The new algorithm, which has been extended towards multivariable systems in Blom & Van den Hof (2010), takes the form of an iterative instrumental variable method, see also Young (1976) and Stoica & Söderström (1981) for earlier results in this direction.

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Although the result in Douma (2006) and Blom & Van den Hof (2010) potentially reduces the number of iterations in frequency-domain identification, a direct implementation of the algorithm exhibits poor numerical properties. This is further supported in this paper, both by means of a theoretical analysis and a numerical example. In fact, the condition numbers associated with the algorithm are quadratically larger than for the standard SK-itertions. This obstructs a reliable and accurate computation of the optimal model. In addition, the approach in Reichel et al. (1991), Van Barel & Bultheel (1995), Van Herpen et al. (2012b) for optimal conditioning of the SK-iterations does not apply to the algorithm in Blom & Van den Hof (2010) due to the lack of an appropriate inner product.

The main contribution of this paper is a new framework for frequency-domain system identification based on a nonlinear least-squares criterion, which i) provides advantageous convergence properties, and ii) ensures optimal numerical conditioning ($\kappa = 1$). Essentially, the proposed solution exploits the results in Blom & Van den Hof (2010), while providing optimal numerical conditioning in the spirit of Reichel et al. (1991), Van Barel & Bultheel (1995), Van Herpen et al. (2012b), albeit through a fundamentally different mechanism. In particular, the new algorithm relies on the introduction of *bi-orthonormal polynomial bases* in system identification. Recently, in Welsh & Goodwin (2003) and Gilson et al. (2013), the need for enhancement of numerical conditioning in frequency-domain instrumental variable identification has been confirmed and some enhancements have been obtained by using an alternative polynomial basis. The approach in this paper reformulates the instrumental-variable algorithm using bi-orthonormal polynomials with respect to a *data-dependent bi-linear form*, which leads to optimal numerical conditioning, i.e., $\kappa = 1$. The following specific contributions are presented in this paper.

(C1) The numerical conditioning that is associated with the linear system of equations of the algorithm in Blom & Van den Hof (2010) is quadratically larger than the condition numbers encountered in the standard SK-iterations (Sanathanan & Koerner, 1963), (Bayard, 1994), (De Callafon et al., 1996), as is shown both theoretically and by means of a numerical example.

(C2) The algorithm in Blom & Van den Hof (2010) has the interpretation of an instrumental variable method. Such type of method admits a transformation of instruments (Söderström & Stoica, 1983). This freedom is exploited to formulate the algorithm in two distinct polynomial bases: one for the model (at the present iteration) and one for the instrument.

(C3) Optimal numerical conditioning is achieved by selecting polynomial bases that are bi-orthonormal with respect to a data-dependent bi-linear form. This bi-linear form accounts for the asymmetric and indefinite character of instrumental variable problems. As a special case, the bi-orthonormal polynomial bases include the orthonormal polynomials with respect to a data-based discrete inner product in Reichel et al. (1991), Van Barel & Bultheel (1995), Van Herpen et al. (2012b).

(C4) Identification of a SISO rational transfer function requires modeling of a numerator and denominator polynomial. Thus, this paper considers a 2×1 vector-polynomial, which is developed in terms of a 2×2 block-polynomial basis. The construction of bi-orthonormal block-polynomials from given frequency response data is presented for continuous-time systems. It is shown that an efficient construction using three-term-recurrence relations is possible, where the recursion coefficients are obtained from a matrix 2×2 block-tridiagonalization problem.

(C5) Superiority of the proposed algorithm is shown by means of a simulation example and is experimentally validated on an industrial motion system.

This paper extends the results in Van Herpen et al. (2012a), in which optimal conditioning of asymmetric polynomial equalities using bi-orthonormal polynomials is introduced, by i) explicitly connecting bi-orthonormal polynomials with instrumental variable identification (C2–C3), and ii) extending the construction of scalar bi-orthormal polynomials towards 2×2 block-polynomials (C4).The latter result facilitates the estimation of a numerator-denominator *vector-polynomial*, which enables a confrontation of the proposed method with frequency-domain identification problems (C5). In Van Herpen (2014, Chap. 2), a complementary study of relevant aspects in the theory of bi-orthonormal polynomials is provided.

This paper is organized as follows. In Sect. 2, the frequency-domain identification problem is posed and two iterative algorithms are compared with respect to their convergence properties. In Sect. 3, the numerical properties of both algorithms are evaluated, motivating the need for enhancement of numerical conditioning (C1). Then, in Sect. 4, bi-orthonormal polynomials are introduced in frequency-domain system identification, which provides optimal numerical conditioning (C2–C3). Subsequently, in Sect. 5, the construction of bi-orthonormal polynomials using three-term-recurrence relations is presented (C4). In Sect. 6, an experimental validation of the benefits of the new algorithm for frequency-domain system identification is provided (C5). Conclusions are drawn in Sect. 7.

Notation: Throughout this paper, ξ represents either $s = \jmath\omega$ or $z = e^{\jmath\omega}$, $\jmath = \sqrt{-1}$, where $\omega \in \mathbb{R}$ denotes a frequency. Moreover, $\mathbb{R}^{p\times q}[\xi]$ denotes a $p \times q$ matrix of real polynomials in ξ. Finally, A^* denotes the conjugate of A, whereas A^H denotes the conjugate transpose of A.

Scope: For clarity of the exposition, attention is restricted to identification of SISO systems. The results in this paper can be generalized to the multivariable situation along conceptually similar lines. In this case, matrix fraction descriptions (MFDs), see, e.g., Kailath (1980, Chap. 6), provide a suitable framework as they directly connect to state-space models. Note that besides model order selection, i.e., the McMillan degree of the model, such multivariable models also require the selection of

Kronecker indices. The reader is referred to Moore (1981) and Gevers (1986) for further information.

In the second part of the paper, the construction of bi-orthonormal block-polynomial bases is presented. Here, attention is restricted to polynomials in the s-domain. The construction of bi-orthornormal block-polynomial bases in the z-domain is conceptually similar.

2. Iterative frequency-domain identification algorithms

2.1. Identification criterion

In this paper, the frequency-domain identification problem $\min_\theta \mathcal{V}(\theta)$ is considered, where

$$\mathcal{V}(\theta) := \sum_{k=1}^{m} \left| W(\xi_k)\,(P_o(\xi_k) \;-\; \hat{P}(\xi_k,\theta)) \right|^2 . \tag{1}$$

In (1), $P_o(\xi_k)$, $k = 1,\ldots,m$, are frequency response function (FRF) measurements of the true system, see Pintelon & Schoukens (2001, Chap. 2) for further details.

The weighting function $W(\xi_k)$ enables a variety of system identification criteria, *cf.* Pintelon et al. (1994) for an overview. Common choices are maximum-likelihood identification (Pintelon & Schoukens, 1990), (McKelvey, 2002) and control-relevant identification (Gevers, 1993), see also Oomen & Bosgra (2008, Sect. VI).

2.2. Model parametrization

The model parametrization that is considered in this paper is

$$\hat{P}(\xi,\theta) = \frac{n(\xi,\theta)}{d(\xi,\theta)}, \tag{2}$$

where $n(\xi,\theta), d(\xi,\theta) \in \mathbb{R}[\xi]$. The numerator and denominator polynomial are formulated as a degree n vector-polynomial

$$\begin{bmatrix} d(\xi,\theta) \\ n(\xi,\theta) \end{bmatrix} = \sum_{j=0}^{n} \varphi_j(\xi)\,\theta_j, \quad \theta = [\theta_0^T \;\theta_1^T \;\cdots\; \theta_n^T]^T. \tag{3}$$

Here, $\theta_j \in \mathbb{R}^{2\times 1}$ and $\varphi_j(\xi) \in \mathbb{R}^{2\times 2}[\xi]$ is of strict degree j, i.e.,

$$\varphi_j(\xi) = \xi^j \cdot s_{jj} \;+\; \ldots \;+\; \xi \cdot s_{j1} \;+\; s_{j0}, \tag{4}$$

where $s_{j0}, s_{j1}, \ldots, s_{jj} \in \mathbb{R}^{2\times 2}$ and s_{jj} is assumed upper triangular and invertible.

In system identification, it is common to let θ_n in (3) be determined by a degree constraint, see also De Moor et al. (1994).

Assumption 1. *In this paper, it is assumed that i) $\hat{P}(\xi,\theta)$ is strictly proper and ii) $d(\xi,\theta)$ is monic. Hence, by virtue of* (4)*,*

$$\theta_n = s_{nn}^{-1}\,[1 \quad 0\,]^T.$$

Example 2. *A common polynomial basis is the monomial basis $\varphi_j^{\mathrm{mon}}(\xi) = \xi^j \cdot I_2$. For this basis,* (3) *corresponds to*

$$\begin{bmatrix} d(\xi,\theta) \\ n(\xi,\theta) \end{bmatrix} = \xi^n \cdot \begin{bmatrix} \theta_{n1} \\ \theta_{n2} \end{bmatrix} + \;\cdots\; + \xi \cdot \begin{bmatrix} \theta_{11} \\ \theta_{12} \end{bmatrix} + \begin{bmatrix} \theta_{01} \\ \theta_{02} \end{bmatrix},$$

where, as a consequence of Assumption 1, $\theta_n = [1 \quad 0\,]^T$.

Due to the model parametrization (2)–(3), criterion (1) is typically non-convex. In the next sections, two iterative algorithms for the minimization of (1) are investigated.

2.3. Traditional iterative algorithm

In this section, the SK-algorithm (Sanathanan & Koerner, 1963) is formulated. Observe that (1) is equivalent to

$$\mathcal{V}(\theta) = \sum_{k=1}^{m} \left| \frac{W(\xi_k)}{d(\xi_k,\theta)} [P_o(\xi_k) \quad -1] \begin{bmatrix} d(\xi_k,\theta) \\ n(\xi_k,\theta) \end{bmatrix} \right|^2. \tag{5}$$

The rationale that motivates the SK-algorithm is that $\mathcal{V}(\theta)$ is convex in θ if $\frac{W(\xi_k)}{d(\xi_k,\theta)}$ is given.

Algorithm I (SK-iteration)**.** *Let $\theta^{\langle 0\rangle}$ be given. In iteration $i = 1,2,\ldots,$ determine the least-squares solution to*

$$\min_{\theta^{\langle i\rangle}} \sum_{k=1}^{m} \left| \frac{W(\xi_k)}{d(\xi_k,\theta^{\langle i-1\rangle})} [P_o(\xi_k) \quad -1] \begin{bmatrix} d(\xi_k,\theta^{\langle i\rangle}) \\ n(\xi_k,\theta^{\langle i\rangle}) \end{bmatrix} \right|^2. \tag{6}$$

By inserting (3), it follows that (6) can be recast as the linear least-squares problem

$$\min_{\vartheta^{\langle i\rangle}} \left\| W_1\,\Phi\,\vartheta^{\langle i\rangle} - b_n \right\|_2^2, \tag{7}$$

where

$$W_1 = \begin{bmatrix} w_{11} & & & \\ & w_{12} & & \\ & & \ddots & \\ & & & w_{1m} \end{bmatrix}, \quad w_{1k} = \frac{W(\xi_k)}{d(\xi_k,\theta^{\langle i-1\rangle})} [P_o(\xi_k) \quad -1], \tag{8}$$

$$\Phi = \begin{bmatrix} \varphi_0(\xi_1) & \varphi_1(\xi_1) & \cdots & \varphi_{n-1}(\xi_1) \\ \varphi_0(\xi_2) & \varphi_1(\xi_2) & \cdots & \varphi_{n-1}(\xi_2) \\ \vdots & \vdots & & \vdots \\ \varphi_0(\xi_m) & \varphi_1(\xi_m) & \cdots & \varphi_{n-1}(\xi_m) \end{bmatrix}, \quad \Phi_n = \begin{bmatrix} \varphi_n(\xi_1) \\ \varphi_n(\xi_2) \\ \vdots \\ \varphi_n(\xi_m) \end{bmatrix}, \tag{9}$$

$$\vartheta^{\langle i\rangle} = \begin{bmatrix} \theta_0^{\langle i\rangle T} & \theta_1^{\langle i\rangle T} & \cdots & \theta_{n-1}^{\langle i\rangle T} \end{bmatrix}^T,$$

and

$$b_n \;=\; -W_1\,\Phi_n\,\theta_n^{\langle i\rangle}. \tag{10}$$

Note that in (7), the vector b_n is determined by the imposed degree constraint, cf. Assumption 1.

Remark 3. *Associated with* (7) *is an orthogonal projection that is defined through the normal equations*

$$(\Phi^H\,W_1^H\,W_1\,\Phi)\,\theta^{\langle i\rangle} \;=\; \Phi^H\,W_1^H\,b_n. \tag{11}$$

Algorithm I is widely applied for frequency-domain system identification (Pintelon et al., 1994). Indeed, the SK-algorithm typically yields a small value of the cost function $\mathcal{V}(\theta)$ in (1). However, the fixed point of the iterations is generally not a (local) optimum of $\mathcal{V}(\theta)$, as is proven in Whitfield (1987).

2.4. Refined iterative algorithm

In this section, a refined iterative algorithm is considered, in which stationary points are a (local) minimum of $\mathcal{V}(\theta)$ in (1). Consider the first order necessary condition for optimality

$$\frac{\partial \mathcal{V}(\theta)}{\partial \theta^T} = 0. \tag{12}$$

Since (1) equals $\mathcal{V}(\theta) = \sum_{k=1}^{m} \varepsilon^H(\xi_k,\theta)\varepsilon(\xi_k,\theta)$, where $\varepsilon(\xi_k,\theta) := W(\xi_k)(P_o(\xi_k) - \hat{P}(\xi_k,\theta))$, (12) equals

$$\sum_{k=1}^{m} \zeta^H(\xi_k,\theta)\,\varepsilon(\xi_k,\theta) \;=\; 0, \tag{13}$$

where

$$\zeta(\xi_k,\theta) := \frac{\partial \varepsilon(\xi_k,\theta)}{\partial \theta^T} = -\,W(\xi_k)\,\frac{\partial \hat{P}(\xi_k,\theta)}{\partial \theta^T}. \tag{14}$$

Thus, a (local) optimum of $\mathcal{V}(\theta)$ is attained when

$$\sum_{k=1}^{m} \left[\frac{-\partial \hat{P}(\xi_k,\theta)}{\partial \theta^T}\right]^H W^H(\xi_k)\,W(\xi_k)\,(P_o(\xi_k) - \hat{P}(\xi_k,\theta)) \;=\; 0. \tag{15}$$

From the model parametrization (2)–(3) it follows that (15) is a nonlinear equality in θ. In order to solve this equality, the following iterative algorithm is proposed in Douma (2006), Blom & Van den Hof (2010).

Algorithm II (IV-iteration)**.** *Let $\theta^{\langle 0\rangle}$ be given. In iteration $i = 1, 2, \ldots$, solve the linear system of equations*

$$\sum_{k=1}^{m} \left[\left.\frac{-\partial \hat{P}(\xi_k,\theta)}{\partial \theta^T}\right|_{\theta=\theta^{\langle i-1\rangle}} \right]^H W^H(\xi_k) \cdot \frac{W(\xi_k)}{d(\xi_k,\theta^{\langle i-1\rangle})} \begin{bmatrix} P_o(\xi_k) & -1 \end{bmatrix} \begin{bmatrix} d(\xi_k,\theta^{\langle i\rangle}) \\ n(\xi_k,\theta^{\langle i\rangle}) \end{bmatrix} \;=\; 0. \tag{16}$$

In the following lemma, (16) is cast in the form of a standard linear system of equations.

Lemma 4. *By inserting* (3) *into* (16)*, the linear system of equations*

$$(\Phi^H\,W_2^H\,W_1\,\Phi)\,\vartheta^{\langle i\rangle} \;=\; \Phi^H\,W_2^H\,b_n \tag{17}$$

is obtained, where W_1, Φ, $\vartheta^{\langle i\rangle}$, and b_n are defined in (8)–(10)*, and*

$$W_2 = \begin{bmatrix} w_{21} & & & \\ & w_{22} & & \\ & & \ddots & \\ & & & w_{2m} \end{bmatrix},\quad w_{2k} = \frac{W(\xi_k)}{d(\xi_k,\theta^{\langle i-1\rangle})}[\hat{P}(\xi_k,\theta^{\langle i-1\rangle}) \quad -1]. \tag{18}$$

***Proof**: By virtue of*

$$\begin{aligned} -\frac{\partial \hat{P}(\xi_k,\theta)}{\partial \theta^T} &= \frac{\partial}{\partial \theta^T}\left(\begin{bmatrix} 0 & \frac{-1}{d(\xi_k,\theta)} \end{bmatrix}\begin{bmatrix} d(\xi_k,\theta) \\ n(\xi_k,\theta) \end{bmatrix}\right) \\ &= \frac{1}{d(\xi_k,\theta)}\begin{bmatrix} \hat{P}(\xi_k,\theta) & -1 \end{bmatrix}\frac{\partial}{\partial \theta^T}\left(\begin{bmatrix} d(\xi_k,\theta) \\ n(\xi_k,\theta) \end{bmatrix}\right), \end{aligned} \tag{19}$$

(14) *equals*

$$\zeta(\xi_k,\theta) = \frac{W(\xi_k)}{d(\xi_k,\theta)}\begin{bmatrix} \hat{P}(\xi_k,\theta) & -1 \end{bmatrix}\begin{bmatrix} \varphi_0(\xi_k)\;\varphi_1(\xi_k)\;\ldots\;\varphi_n(\xi_k) \end{bmatrix}. \tag{20}$$

Then, (17) *follows after writing* (16) *in matrix form, where b_n follows from the degree constraint in Assumption 1.* ■

Remark 5. *Note that the system of equations* (17) *represents an* oblique*, i.e.,* non-orthogonal*, projection.*

Compared to Alg. I, the essential advantage of Alg. II is that upon convergence, it is guaranteed that a (local) optimum of $\mathcal{V}(\theta)$ in (1) is attained. In the forthcoming section, the numerical properties of both algorithms are investigated.

3. Numerical analysis of the iterative algorithms

The iterative frequency-domain identification algorithms that are presented in Sect. 2 both rely on solving a linear system of equations of the form $Ax = b$. The accuracy of the solution in each iteration is determined by the condition number $\kappa(A)$ (Golub & Van Loan, 1989, Sect. 5.3.7), which is defined as

$$\kappa(A) = \overline{\sigma}(A) \,/\, \underline{\sigma}(A).$$

In this section, the numerical conditioning associated with Alg. I and Alg. II is further investigated.

3.1. Numerical ill-conditioning: increased importance for the IV-algorithm

In this section, it is shown that the use of a standard polynomial basis in Alg. II can lead to extremely large condition numbers, which obstructs a reliable implementation of the algorithm. This forms the theoretical aspect of Contribution C1.

First the SK-iteration in Alg. I is considered, in which (7) is the essential computational step. In each iteration, the least-squares solution to

$$W_1\,\Phi\,\vartheta^{\langle i\rangle} \;=\; b_n \tag{21}$$

is computed, with the associated condition number $\kappa(W_1\,\Phi)$. This condition number crucially depends on the choice of polynomial basis in (3). A common choice is the monomial basis, which is applied in, e.g., Bayard et al. (1991), De Callafon et al. (1996). However, this typically leads to $\kappa(W_1\,\Phi) \gg 1$, as is illustrated next.

Example 6. *Consider $\varphi_j^{\mathrm{mon}}(\xi) = \xi^j \cdot I_2$, $j = 0, 1, \ldots, n$, see Example 2. Then,* (9) *yields the block-Vandermonde matrix*

$$\Phi^{\mathrm{mon}} = \begin{bmatrix} I_2 & \xi_1 \cdot I_2 & \ldots & \xi_1^{n-1} \cdot I_2 \\ I_2 & \xi_2 \cdot I_2 & \ldots & \xi_2^{n-1} \cdot I_2 \\ \vdots & \vdots & & \vdots \\ I_2 & \xi_m \cdot I_2 & \ldots & \xi_m^{n-1} \cdot I_2 \end{bmatrix}.$$

Now, let $\xi_k = \jmath \cdot 2\pi \cdot \{1, 10, 100, 1000\}$ and $n = 3$. Then, $\kappa(\Phi^{\mathrm{mon}}) = 3.0 \cdot 10^7 \gg 1$.

Example 6 motivates for frequency points on the imaginary axis, or non-equidistantly spaced frequency points on the unit circle, that the use of the monomial basis typically leads to $\kappa(W_1\,\Phi) \gg 1$ (assuming $W_1 = I$). In other words, (21) is typically numerically ill-conditioned, leading to an inaccurate numerical solution of Alg. I (in a worst-case sense).

Next, consider Alg. II, with the system of equations (17) as key computational step. The solution accuracy depends on $\kappa(\Phi^H\,W_2^H\,W_1\,\Phi)$. The following result reveals that this condition number is quadratically worse than $\kappa(W_1\,\Phi)$, associated with the SK-algorithm.

Result 7. *Consider the desired situation where upon convergence of Alg. II, $\hat{P}(\xi_k,\theta^\star) \approx P_o(\xi_k)$, $k = 1, \ldots, m$, where $\theta^\star$ denotes a fixed point of the iterations* (16)*. In that case, $W_2 \approx W_1$, cf.* (8) *and* (18)*. As a result,*

$$\kappa(\Phi^H\,W_2^H\,W_1\,\Phi) \;\approx\; \kappa(\Phi^H\,W_1^H\,W_1\,\Phi) \;=\; \kappa(W_1\Phi)^2. \tag{22}$$

Result 7 reveals that the use of monomial basis polynomials in Alg. II, as considered in Blom & Van den Hof (2010), potentially leads to a severely ill-conditioned system of equations (17).

Remark 8. *In view of* (22)*, it is favorable to solve the least squares problem* (7) *through QR-factorization of* $W_1\Phi$ *in* (21)*, instead of solving the normal equations* (11)*, see also (Golub & Van Loan, 1989, Sect. 5.3.8). However, this approach does not apply to the oblique projection* (17)*.*

3.2. Classical solutions for improvement of conditioning: limitations on applicability to the IV-algorithm

In Sect. 3.1, it was shown that the use of the monomial polynomial basis leads to very bad numerical conditioning of Alg. I and especially of Alg. II. In the literature, several approaches have been considered to mitigate the conditioning problems in frequency-domain system identification, including

i) discarding the least-relevant part of the system of equations, e.g., by means of a singular-value decomposition (Wills & Ninness, 2008),

ii) amplitude scaling (Hakvoort & Van den Hof, 1994),

iii) frequency scaling (Pintelon & Kollár, 2005),

iv) conversion from the continuous-time domain to the discrete-time domain and vice-versa using a Möbius transformation (Oomen et al., 2007, Sect. 5.1), and

v) the use of an alternative classical polynomial basis such as Chebyshev polynomials (Dailey & Lukich, 1987), (Adcock, 1987), the use of basis functions that are orthonormal with respect to the standard inner product in the Hilbert space $\mathcal{RH}_2$ (De Vries & Van den Hof, 1998), (Heuberger et al., 2005), or the use of frequency localising basis functions (FLBFs) that have been proposed recently in Welsh & Goodwin (2003), Gilson et al. (2013).

Although the mentioned approaches often help in mitigating the numerical ill-conditioning, they typically require heuristic tuning and may not provide sufficient improvement for complex frequency-domain identification problems.

Furthermore, for the classical Alg. I, a fundamental solution to prevent numerical ill-conditioning of (21) exists. It relies on the use of a *data-dependent* polynomial basis, in which the following inner product plays an important role.

Definition 9. *Let distinct frequency points* $\xi_k \in \mathbb{C}$, $k = 1, \ldots, m$, *be given. Let* $w_{1k} \in \mathbb{C}^{1\times 2}$ *be weights as specified in* (8)*. Then, for vector polynomials* $\phi_i(\xi), \phi_j(\xi) \in \mathbb{R}^{2\times 1}[\xi]$ *the following data-dependent inner product is defined:*

$$\langle \phi_i(\xi),\ \phi_j(\xi)\rangle \ := \ \sum_{k=1}^{m} \phi_j^H(\xi_k)\, w_{1k}^H\, w_{1k}\, \phi_i(\xi_k). \tag{23}$$

As shown in Reichel et al. (1991), Van Barel & Bultheel (1995), Faßbender (1997), if a polynomial basis is *orthonormal* with respect to (23), then in (11) it holds that

$$\Phi^H W_1^H W_1 \Phi = I_{2n}\,.$$

Equivalently, $\kappa(W_1\,\Phi) = 1$ in (21). Hence, optimal conditioning is achieved, facilitating a numerically reliable implementation of Alg. I.

Although a polynomial basis that is orthonormal with respect to (23) provides optimal conditioning of the SK-iteration in Alg. I, this does not apply to Alg. II. Importantly, whereas $\kappa(W_1\,\Phi) = 1$, in contrast, $\kappa(\Phi^H\, W_2^H\, W_1\,\Phi)$ can be arbitrarily large for general data. The underlying reason is that the *oblique* projection (17) is not associated with an inner product of the form in Def. 9. In fact, it is shown in Van Herpen (2014, Chap. 2, Thm. 2.19) that if

$$\exists\ k = 1, \ldots, m, \quad \text{s.t.} \quad w_{2k}^H w_{1k} \ \neq\ w_{1k}^H w_{2k}\,,$$

i.e., $W_2^H W_1$ is asymmetric, then (disregarding some degenerate cases) it is not possible to select *one single* polynomial basis $\varphi_j(\xi)$, $j = 0, 1, \ldots, n-1$, that yields $\kappa(\Phi^H\, W_2^H\, W_1\,\Phi) = 1$.

In conclusion, whereas Alg. II has beneficial convergence properties compared to Alg. I, the existing approaches for implementation of this algorithm do not provide optimal numerical conditioning. In the forthcoming section, a new solution is presented that does provide optimal conditioning in Alg. II.

4. Optimally conditioned frequency-domain IV-identification using bi-orthonormal polynomial bases

In this section, a new solution is presented that combines the algorithmic advantages of Alg. II with optimal numerical conditioning. As observed in Blom & Van den Hof (2010), $\zeta(\xi, \theta)$ in (14) can be interpreted as an instrumental variable (IV), see Söderström & Stoica (1983) for an overview of instrumental variable methods in system identification. In this section, it is shown that through a coordinate transformation of the instrumental variable problem, and by the introduction of bi-orthonormal polynomials in system identification, it is possible to achieve optimal numerical conditioning in Alg. II, such that $\kappa = 1$. This forms Contributions C2 and C3 of this paper.

4.1. Additional freedom by a static transformation of instruments

The essential difference between the identification algorithms considered in this paper is that Alg. I relies on the orthogonal projection (11), in which $\Phi^H W_1^H W_1 \Phi$ is symmetric, whereas Alg. II is based on the oblique projection (17), in which $\Phi^H W_2^H W_1 \Phi$ is an *asymmetric*, indefinite matrix, see also Gohberg et al. (2005) for a treatment on indefinite linear algebra. Consequently, a polynomial basis that is orthonormal with respect to an inner product of the form (23) does not lead to optimal results in Alg. II. To obtain optimal numerical conditioning, the asymmetric character of Alg. II has to be accounted for explicitly. To this end, the algorithm is reformulated in a more general form in which *two distinct* polynomial bases are used.

Definition 10. *In analogy to* (4)*, a basis* $\psi_j(\xi) \in \mathbb{R}^{2\times 2}[\xi]$, $j = 0, 1, \ldots, n$, *is defined, where* $\psi_j(\xi)$ *is of strict degree* j*, viz.*

$$\psi_j(\xi) = \xi^j \cdot t_{jj} \ + \ \ldots \ + \ \xi \cdot t_{j1} \ + \ t_{j0}, \tag{24}$$

with $t_{jk} \in \mathbb{R}^{2\times 2}$, $k = 0, \ldots, j$. In addition, t_{jj} is assumed to be upper triangular and invertible.

Definition 11. *Consider the two polynomial bases $\varphi_j(\xi)$, $\psi_j(\xi)$, $j = 0, 1, \ldots, n$, in* (4) *and* (24)*. Then, the coefficient matrices $S, T \in \mathbb{R}^{2(n+1)\times 2(n+1)}$ are defined as*

$$S = \begin{bmatrix} s_{00} & s_{10} & \ldots & s_{n0} \\ & s_{11} & \ldots & s_{n1} \\ & & \ddots & \vdots \\ & & & s_{nn} \end{bmatrix}, \quad T = \begin{bmatrix} t_{00} & t_{10} & \ldots & t_{n0} \\ & t_{11} & \ldots & t_{n1} \\ & & \ddots & \vdots \\ & & & t_{nn} \end{bmatrix}.$$

Note that S and T are upper triangular and invertible. The following auxiliary result now follows immediately.

Result 12. *The unique static transformation from the polynomial basis $\varphi_j(\xi)$ in* (4) *to the basis $\psi_j(\xi)$ in Def. 10 is given by*

$$\begin{bmatrix} \psi_0(\xi) & \psi_1(\xi) & \cdots & \psi_n(\xi) \end{bmatrix} = \begin{bmatrix} \varphi_0(\xi) & \varphi_1(\xi) & \cdots & \varphi_n(\xi) \end{bmatrix} U,$$

with $U = S^{-1}T \in \mathbb{R}^{2(n+1)\times 2(n+1)}$ upper triangular and invertible.

In the remainder of this section, a more general formulation of the instrumental variable identification problem in Alg. II is derived. Herein, the *two distinct* polynomial bases $\varphi(\xi)$ and $\psi(\xi)$ are exploited. In particular, a specific transformation of the instruments is performed, which has the interpretation of a change of polynomial basis. The forthcoming developments lead to the main result in Lemma 13.

Consider Alg. II, where $\hat{P}(\varphi(\xi), \theta^{\langle i-1\rangle}) = \dfrac{n(\varphi(\xi), \theta^{\langle i-1\rangle})}{d(\varphi(\xi), \theta^{\langle i-1\rangle})}$ is the model obtained in iteration $(i-1)$, with

$$\begin{bmatrix} d(\varphi(\xi), \theta^{\langle i-1\rangle}) \\ n(\varphi(\xi), \theta^{\langle i-1\rangle}) \end{bmatrix} = \begin{bmatrix} \varphi_0(\xi) & \varphi_1(\xi) & \cdots & \varphi_n(\xi) \end{bmatrix} \theta^{\langle i-1\rangle}$$

Here, the parametrization in the basis $\varphi(\xi)$, see (3), is indicated explicitly. Using Result 12, the model is re-parameterized in an alternative basis $\psi_j(\xi)$, $j = 0, 1, \ldots n$, which leads to $\hat{P}(\psi(\xi), \eta^{\langle i-1\rangle})$. Here, $\eta^{\langle i-1\rangle} = U^{-1}\,\theta^{\langle i-1\rangle}$ is the parameter vector that provides the same model in the new basis $\psi(\xi)$, i.e.,

$$\begin{bmatrix} d(\varphi(\xi), \theta^{\langle i-1\rangle}) \\ n(\varphi(\xi), \theta^{\langle i-1\rangle}) \end{bmatrix} = \begin{bmatrix} d(\psi(\xi), \eta^{\langle i-1\rangle}) \\ n(\psi(\xi), \eta^{\langle i-1\rangle}) \end{bmatrix} = \begin{bmatrix} \psi_0(\xi) & \psi_1(\xi) & \cdots & \psi_n(\xi) \end{bmatrix} \eta^{\langle i-1\rangle}$$

In accordance with (19), it now follows that

$$\begin{aligned} & -\left.\frac{\partial \hat{P}(\psi(\xi), \eta)}{\partial \eta^T}\right|_{\eta=\eta^{\langle i-1\rangle}} \qquad (25) \\ &= \frac{1}{d(\psi(\xi), \eta^{\langle i-1\rangle})} \begin{bmatrix} \hat{P}(\psi(\xi), \eta^{\langle i-1\rangle}) & -1 \end{bmatrix} \cdot \frac{\partial}{\partial \eta^T} \left(\begin{bmatrix} d(\psi(\xi), \eta) \\ n(\psi(\xi), \eta) \end{bmatrix} \right) \\ &= \frac{1}{d(\varphi(\xi), \theta^{\langle i-1\rangle})} \begin{bmatrix} \hat{P}(\varphi(\xi), \theta^{\langle i-1\rangle}) & -1 \end{bmatrix} \cdot \begin{bmatrix} \psi_0(\xi) & \psi_1(\xi) & \ldots & \psi_n(\xi) \end{bmatrix}, \end{aligned}$$

which represents the gradient of the model $\hat{P}(\xi, \theta^{\langle i-1\rangle})$ when evaluated in terms of the polynomial basis $\psi_j(\xi)$, $j = 0, 1, \ldots n$. Note that this new basis $\psi_j(\xi)$ only appears explicitly as the *rightmost matrix* in the product (25). The remaining two terms can still be evaluated in terms of the basis $\varphi_j(\xi)$, as is done (implicitly) in (19).

In the following lemma, *two distinct* polynomial bases are used to parameterize the model and the instrumental variable. This constitutes Contribution C2 of the paper.

Lemma 13. *Consider* (16)*, where*

i) vector-polynomial $[d(\xi, \theta^{\langle i\rangle}) \;\; n(\xi, \theta^{\langle i\rangle})]^T$ is formulated in the polynomial basis $\varphi_j(\xi)$, cf. (3)*,*

ii) instrumental variable $\zeta(\xi, \theta^{\langle i-1\rangle}) = -W(\xi) \cdot \left.\frac{\partial \hat{P}(\xi,\theta)}{\partial \theta}\right|_{\theta=\theta^{\langle i-1\rangle}}$, see (14)*, is evaluated for a* different *basis $\psi_j(\xi)$, i.e., using the result in* (25)*,*

$$\begin{aligned} & \tilde{\zeta}(\xi, \theta^{\langle i-1\rangle}) \qquad (26) \\ & := \frac{W(\xi_k)}{d(\xi_k, \theta^{\langle i-1\rangle})} \begin{bmatrix} \hat{P}(\xi_k, \theta^{\langle i-1\rangle}) & -1 \end{bmatrix} \begin{bmatrix} \psi_0(\xi_k) & \psi_1(\xi_k) & \ldots & \psi_n(\xi_k) \end{bmatrix}. \end{aligned}$$

Then, the solution $\theta^{\langle i\rangle}$ to

$$\sum_{k=1}^{m} \tilde{\zeta}^H(\xi_k, \theta^{\langle i-1\rangle}) \cdot \frac{W(\xi_k)}{d(\xi_k, \theta^{\langle i-1\rangle})} \begin{bmatrix} P_o(\xi_k) & -1 \end{bmatrix} \begin{bmatrix} d(\xi_k, \theta^{\langle i\rangle}) \\ n(\xi_k, \theta^{\langle i\rangle}) \end{bmatrix} = 0. \qquad (27)$$

is equivalent to the solution $\theta^{\langle i\rangle}$ to (16)*.*

Proof: *By virtue of Result 12, $\tilde{\zeta}(\xi_k, \theta) = \zeta(\xi_k, \theta)U$, see* (20) *and* (26)*. Since U is invertible, the solution θ to*

$$\sum_{k=1}^{m} \tilde{\zeta}^H(\xi_k, \theta)\, \varepsilon(\xi_k, \theta) = 0,$$

is equivalent to the solution θ to (13)*. In analogy to this, the solution $\theta^{\langle i\rangle}$ to* (27) *and* (16) *is equivalent.* ■

Remark 14. *A transformation of the polynomial basis in which $\zeta(\xi, \theta)$ is evaluated constitutes a special form of a* transformation of instruments*. Indeed, the parameter estimation in instrumental variable system identification problems is invariant under a linear transformation of instruments, as is also shown in Söderström & Stoica (1983, Sect. 3.1, pp. 24–25).*

The rationale behind Lemma 13 is that by evaluating the instrumental variable $\zeta(\xi, \theta)$ in terms of a different polynomial basis, additional freedom is provided to formulate the system of equations in Alg. II. In particular, it follows along the lines of Lemma 4 that it is possible to recast (27) as

$$(\Psi^H\, W_2^H\, W_1\, \Phi)\, \vartheta^{\langle i\rangle} = \Psi^H\, W_2^H\, b_n, \qquad (28)$$

where W_1, W_2, Φ, $\vartheta^{\langle i\rangle}$, and b_n are defined in (8)–(10) and (18), and

$$\Psi = \begin{bmatrix} \psi_0(\xi_1) & \psi_1(\xi_1) & \cdots & \psi_{n-1}(\xi_1) \\ \psi_0(\xi_2) & \psi_1(\xi_2) & \cdots & \psi_{n-1}(\xi_2) \\ \vdots & \vdots & & \vdots \\ \psi_0(\xi_m) & \psi_1(\xi_m) & \cdots & \psi_{n-1}(\xi_m) \end{bmatrix}.$$

In the next section, the freedom in (28) when compared to (17) is exploited to achieve optimal numerical conditioning in frequency-domain instrumental variable identification, see Alg. II.

4.2. Bi-orthonormal polynomial bases for optimally conditioned frequency-domain system identification

In this section, optimal numerical conditioning of Alg. II is achieved through the introduction of bi-orthonormal polynomials in system identification. To this end, a *data-dependent* bi-linear form is introduced.

Definition 15. *Let distinct frequency points $\xi_k \in \mathbb{C}$, $k = 1, \ldots, m$, be given. Let $w_{1k}, w_{2k} \in \mathbb{C}^{1\times 2}$ be weights as defined in* (8) *and* (18)*. For* vector-*polynomials $\underline{\varphi}(\xi), \underline{\psi}(\xi) \in \mathbb{R}^{2\times 1}[\xi]$, the data-dependent bi-linear form $[\cdot,\ \cdot]$ is defined as*

$$[\underline{\varphi}(\xi),\ \underline{\psi}(\xi)] \ := \ \sum_{k=1}^{m} \underline{\psi}^H(\xi_k)\, w_{2k}^H\, w_{1k}\, \underline{\varphi}(\xi_k). \tag{29}$$

Remark 16. *Note that* (29) *is not an inner product, since in general this bi-linear form is asymmetric and indefinite, see Van Herpen (2014, Sect. 2.3). In the special situation where $w_{1k} = w_{2k}\ \forall\, k = 1, \ldots, m$, then* (29) *reduces to the data-dependent inner product* (23)*.*

Definition 17. *For* block-*polynomials $\varphi(\xi), \psi(\xi) \in \mathbb{R}^{2\times 2}[\xi]$, a generalization of* (29) *is given by*

$$[\![\varphi(\xi),\ \psi(\xi)]\!] := \sum_{k=1}^{m} \psi^H(\xi_k)\, w_{2k}^H\, w_{1k}\, \varphi(\xi_k). \tag{30}$$

Indeed, let $\varphi(\xi)$ be decomposed into vector-polynomials

$$\varphi(\xi) = [\underline{\varphi}_1(\xi)\ \ \underline{\varphi}_2(\xi)], \quad \underline{\varphi}_1, \underline{\varphi}_2 \in \mathbb{R}^{2\times 1}[\xi],$$

and similarly for $\psi(\xi)$. Then, element (e_2, e_1) in (30)*, where $e_1, e_2 \in \{1, 2\}$, is given by the bi-linear form $[\underline{\varphi}_{e_1}(\xi), \underline{\psi}_{e_2}(\xi)]$.*

The following theorem is the main result of this section and constitutes Contribution C3 of the paper. Here, the freedom to choose two different polynomial bases in frequency-domain instrumental variable identification, cf. Lemma 13, is exploited.

Theorem 18. *Consider* (28)*. Let $\varphi_i(\xi), \psi_j(\xi)$, $i, j = 0, 1, \ldots, n-1$ be bi-orthonormal with respect to* (30)*, i.e.*

$$[\![\varphi_i(\xi),\ \psi_j(\xi)]\!] \ = \ \delta_{ij} \cdot I_2, \quad i, j = 0, 1, \ldots, n-1. \tag{31}$$

Then, $\kappa(\Psi^H\, W_2^H\, W_1\, \Phi) = 1$.

Proof: *The result follows by observing that* (31) *in matrix form reads*

$$\Psi^H\, W_2^H\, W_1\, \Phi = I_{2n},$$

hence, $\kappa(\Psi^H\, W_2^H\, W_1\, \Phi) = 1$. ■

Theorem 18 reveals that when bi-orthonormal polynomials (BPs) with respect to (30) are used, optimal numerical conditioning of (28) is achieved. Hence, the key computational step in Alg. II is optimally conditioned, which facilitates a reliable implementation of the algorithm. In the next section, the construction of BPs with respect to (30) is considered.

5. Construction of bi-orthonormal block-polynomial bases

In this section, the construction of a set of polynomial bases that are bi-orthonormal with respect to the bi-linear form (30) is considered. This constitutes Contribution C4 of the paper.

To facilitate the exposition, the polynomial bases $\varphi_j(\xi), \psi_j(\xi)$, $j = 0, 1, \ldots, n-1$, as well as the weights w_{1k}, w_{2k}, $k = 1, \ldots, m$, are initially assumed to be *scalar*. It is then explained how to construct $\varphi_j(\xi), \psi_j(\xi)$ that are bi-orthonormal with respect to the *scalar* bi-linear form

$$[\varphi(\xi),\ \psi(\xi)] \ = \ \sum_{k=1}^{m} \varphi^*(\xi_k)\, w_{2k}^*\, w_{1k}\, \varphi(\xi_k). \tag{32}$$

In Sect. 5.8, the presented concepts are generalized towards the construction of *block-polynomials* that are bi-linear with respect to (30).

5.1. Polynomial recurrence relations

Throughout this section, polynomial bases that satisfy a degree structure are considered. In analogy with (4) and (24), the scalar polynomials $\varphi_j(\xi), \psi_j(\xi)$ take the form

$$\begin{aligned} \varphi_j(\xi) \ &= \ \xi^j \cdot s_{jj} \ + \ \ldots \ + \ \xi \cdot s_{j1} \ + \ s_{j0}, \\ \psi_j(\xi) \ &= \ \xi^j \cdot t_{jj} \ + \ \ldots \ + \ \xi \cdot t_{j1} \ + \ t_{j0}, \end{aligned}$$

where s_{jk}, t_{jk}, $k = 0, 1, \ldots, j$, are scalars. In addition, s_{jj} and t_{jj} are assumed to be nonzero, such that the j^{th} polynomial is of strict degree j. As a consequence of the imposed degree structure, scalars $\sigma_{k,j-1}, \tau_{k,j-1}$, $k = 0, 1, \ldots, j$, exist such that

$$\xi\, \varphi_{j-1}(\xi) = \varphi_j(\xi)\, \sigma_{j,j-1} + \cdots + \varphi_1(\xi)\, \sigma_{1,j-1} + \varphi_0(\xi)\, \sigma_{0,j-1}, \tag{33}$$
$$\xi\, \psi_{j-1}(\xi) = \psi_j(\xi)\, \tau_{j,j-1} + \cdots + \psi_1(\xi)\, \tau_{1,j-1} + \psi_0(\xi)\, \tau_{0,j-1}. \tag{34}$$

Now, let $n = m$, i.e., consider as many basis polynomials as the number of data points that define the bi-linear form (32). Then, combining (33)–(34) for $j = 0, 1, \ldots, n-1$ yields

$$\begin{aligned} &\xi \begin{bmatrix} \varphi_0(\xi) & \varphi_1(\xi) & \cdots & \varphi_{m-1}(\xi) \end{bmatrix} \ = \\ &\begin{bmatrix} \varphi_0(\xi) & \varphi_1(\xi) & \cdots & \varphi_{m-1}(\xi) \end{bmatrix} H_1 \ + \ \varphi_m(\xi) \begin{bmatrix} 0_{1\times(m-1)} & \sigma_{m,m-1} \end{bmatrix}, \end{aligned} \tag{35}$$

$$\begin{aligned} &\xi \begin{bmatrix} \psi_0(\xi) & \psi_1(\xi) & \cdots & \psi_{m-1}(\xi) \end{bmatrix} \ = \\ &\begin{bmatrix} \psi_0(\xi) & \psi_1(\xi) & \cdots & \psi_{m-1}(\xi) \end{bmatrix} H_2 \ + \ \psi_m(\xi) \begin{bmatrix} 0_{1\times(m-1)} & \tau_{m,m-1} \end{bmatrix}, \end{aligned} \tag{36}$$

where

$$H_1 = \begin{bmatrix} \sigma_{00} & \cdots & \sigma_{0,m-2} & \sigma_{0,m-1} \\ \sigma_{10} & \cdots & \sigma_{1,m-2} & \sigma_{1,m-1} \\ & \ddots & \vdots & \vdots \\ & & \sigma_{m-1,m-2} & \sigma_{m-1,m-1} \end{bmatrix}, \tag{37}$$

$$H_2 = \begin{bmatrix} \tau_{00} & \cdots & \tau_{0,m-2} & \tau_{0,m-1} \\ \tau_{10} & \cdots & \tau_{1,m-2} & \tau_{1,m-1} \\ & \ddots & \vdots & \vdots \\ & & \tau_{m-1,m-2} & \tau_{m-1,m-1} \end{bmatrix}, \tag{38}$$

are upper Hessenberg matrices. To let the recurrence relations (35)–(36) generate *bi-orthonormal polynomials with respect to* (32)*,* the specific problem data has to be introduced into the recurrence coefficients in the Hessenberg matrix. Before presenting the key results, several auxiliary matrix definitions are introduced.

5.2. Auxiliary matrix definitions

The bi-linear form (32) is based on m frequency points $\xi_k, k = 1, \ldots, m$, with corresponding weights w_{1k}, w_{2k}. Denote matrices

$$\begin{aligned} X &= \text{diag}(\xi_1, \xi_2, \ldots, \xi_m) \in \mathbb{C}^{m\times m}, \\ W_1 &= \text{diag}(w_{11}, w_{12}, \ldots, w_{1m}) \in \mathbb{C}^{m\times m}, \\ W_2 &= \text{diag}(w_{21}, w_{22}, \ldots, w_{2m}) \in \mathbb{C}^{m\times m}. \end{aligned} \tag{39}$$

Also, denote vectors

$$\underline{w}_1 = \begin{bmatrix} w_{11} & w_{12} & \ldots & w_{1m} \end{bmatrix}^T \in \mathbb{C}^{m\times 1}, \tag{40}$$

$$\underline{w}_2 = \begin{bmatrix} w_{21} & w_{22} & \ldots & w_{2m} \end{bmatrix}^T \in \mathbb{C}^{m\times 1}. \tag{41}$$

Finally, denote

$$\Phi = \begin{bmatrix} \Phi_0 & \Phi_1 & \cdots & \Phi_{m-1} \end{bmatrix} = \begin{bmatrix} \varphi_0(\xi_1) & \varphi_1(\xi_1) & \cdots & \varphi_{m-1}(\xi_1) \\ \varphi_0(\xi_2) & \varphi_1(\xi_2) & \cdots & \varphi_{m-1}(\xi_2) \\ \vdots & \vdots & & \vdots \\ \varphi_0(\xi_m) & \varphi_1(\xi_m) & \cdots & \varphi_{m-1}(\xi_m) \end{bmatrix} \in \mathbb{C}^{m\times m},$$

$$\Psi = \begin{bmatrix} \Psi_0 & \Psi_1 & \cdots & \Psi_{m-1} \end{bmatrix} = \begin{bmatrix} \psi_0(\xi_1) & \psi_1(\xi_1) & \cdots & \psi_{m-1}(\xi_1) \\ \psi_0(\xi_2) & \psi_1(\xi_2) & \cdots & \psi_{m-1}(\xi_2) \\ \vdots & \vdots & & \vdots \\ \psi_0(\xi_m) & \psi_1(\xi_m) & \cdots & \psi_{m-1}(\xi_m) \end{bmatrix} \in \mathbb{C}^{m\times m}.$$

For scalar polynomials, bi-orthormality condition (31) reduces to $[\varphi_i(\xi), \psi_j(\xi)] = \delta_{ij}$, $i, j = 0, 1, \ldots, n-1$, where (32) is used. This bi-orthonormality condition is equivalent to the matrix representation

$$\Psi^H W_2^H W_1 \Phi = I_m. \tag{42}$$

In Sect. 5.3–Sect. 5.7, the matrices X, W_1, W_2, and $\underline{w}_1, \underline{w}_2$, and Φ, Ψ are assumed to be dimensioned accordingly.

5.3. Connecting the polynomial recurrences with the data: a requirement on the eigenvalues of the Hessenberg matrices

The general j-term recurrence relations (35)–(36) hold for *any* polynomial bases $\varphi_j(\xi), \psi_j(\xi)$ with the assumed degree structure. In this section, an additional requirement on the Hessenberg matrices H_1 and H_2 is formulated that needs to be fulfilled to let $\varphi_j(\xi), \psi_j(\xi)$ be bi-orthonormal with respect to (32). For this purpose, observe that if $\varphi_j(\xi), \psi_j(\xi)$ are bi-orthonormal polynomials, then (35)–(36) have a specific form.

Lemma 19. *Let $\varphi_j(\xi), \psi_j(\xi)$, $j = 0, 1, \ldots, n-1$, be bi-orthonormal polynomials with respect to* (32)*, where $n = m$. Then,* (35)–(36) *are equivalent to*

$$X\Phi = \Phi H_1, \tag{43}$$

$$X\Psi = \Psi H_2. \tag{44}$$

Proof: *The bi-linear form* (32) *is based on the frequency points $\xi_k, k = 1, \ldots, m$. Evaluating* (35)–(36) *for these frequencies yields*

$$\begin{aligned} X\Phi &= \Phi H_1 + \Phi_m \begin{bmatrix} 0_{1\times(m-1)} & \sigma_{m,m-1} \end{bmatrix}, \\ X\Psi &= \Phi H_2 + \Psi_m \begin{bmatrix} 0_{1\times(m-1)} & \tau_{m,m-1} \end{bmatrix}, \end{aligned}$$

where

$$\begin{aligned} \Phi_m &= \begin{bmatrix} \varphi_m(\xi_1) & \varphi_m(\xi_2) & \cdots & \varphi_m(\xi_m) \end{bmatrix}^T \\ \Psi_m &= \begin{bmatrix} \psi_m(\xi_1) & \psi_m(\xi_2) & \cdots & \varphi_m(\xi_m) \end{bmatrix}^T. \end{aligned}$$

Since it is assumed that the m frequency points are distinct, it follows as a consequence of the imposed polynomial degree structure that Φ and Ψ are invertible matrices. Hence, in order for $\varphi_m(\xi), \psi_m(\xi)$ to be bi-orthogonal with all lower degree basis polynomials, it is required that $\varphi_m(\xi_k) = \psi_m(\xi_k) = 0 \; \forall \; \xi_k$. Thus, $\Phi_m = \Psi_m = 0_{m\times 1}$, proving (43)–(44)*.* ■

Using a bi-linear form based on m distinct frequency points, *bi-orthonormal* bases $\varphi_j(\xi), \psi_j(\xi)$ of m non-trivial polynomials can be obtained. The relations (43)–(44) describe the relations between these polynomials for the frequencies on which the bi-linear form is defined. It turns out that the Hessenberg matrices H_1 and H_2 have precisely these frequencies as its eigenvalues.

Theorem 20. *Let $\varphi_j(\xi), \psi_j(\xi)$, $j = 0, 1, \ldots, n-1$, be bi-orthonormal polynomials with respect to* (32)*, where $n = m$. Then,* (43)–(44) *are equivalent to*

$$(\Psi^H W_2^H) X (W_1 \Phi) = H_1, \tag{45}$$

$$(\Phi^H W_1^H) X (W_2 \Psi) = H_2, \tag{46}$$

where

$$\Psi^H W_2^H = (W_1 \Phi)^{-1}. \tag{47}$$

Proof: *Consider the bi-orthonormality condition* (42)*, which immediately yields* (47)*. Next,* (45)–(46) *follow after pre-multiplication of* (43) *and* (44) *by $(\Psi^H W_2^H) W_1$ and $(\Phi^H W_1^H) W_2$, respectively.* ■

Theorem 20 shows that the Hessenberg matrices H_1 and H_2 are similar to X. Consequently, the eigenvalues of both H_1 and H_2 are ξ_k, $k = 1, \ldots, m$. Indeed, bi-orthonormal polynomials can be constructed by solving two *inverse* eigenvalue problems. Before showing this, the lowest degree polynomial is appropriately selected to initialize the recurrence relations.

5.4. Requirement for initialization of bi-orthonormal bases

Recall from Sect. 5.1 that H_1 and H_2 contain the recurrence coefficients that relate basis polynomials of increasing degree. The associated recurrence relations are given by (43)–(44). The

missing aspect for the actual construction of bi-orthonormal polynomials is the *initialization of the polynomial bases*. The following result enables initialization of the polynomial bases from the bi-linear form (32).

Theorem 21. *Let $\varphi_j(\xi), \psi_j(\xi)$, $j = 0, 1, \ldots, n-1$ be bi-orthonormal polynomials with respect to* (32)*, where $n = m$. Furthermore, let the* 0^{th} *degree basis polynomials be defined as*

$$\varphi_0(\xi) \;:=\; \frac{1}{\gamma_0}, \qquad \psi_0(\xi) \;:=\; \frac{1}{\beta_0}, \tag{48}$$

where β_0 and γ_0 are scalars. Then, since $\varphi_0(\xi)$ and $\psi_0(\xi)$ are part of bi-orthonormal polynomial bases, the following equalities hold:

$$(\Psi^H\, W_2^H)\, \underline{w}_1 \;=\; \begin{bmatrix}\gamma_0 & 0_{1,m-1}\end{bmatrix}^T, \tag{49}$$

$$(\Phi^H\, W_1^H)\, \underline{w}_2 \;=\; \begin{bmatrix}\beta_0 & 0_{1,m-1}\end{bmatrix}^T. \tag{50}$$

Proof: *Let $\varphi_0(\xi)$ and $\psi_0(\xi)$ be as defined in* (48)*. From the auxiliary matrix definitions in Sect. 5.2, it follows that*

$$W_1\, \Phi_0 \;=\; \underline{w}_1\, \frac{1}{\gamma_0}, \tag{51}$$

$$W_2\, \Psi_0 \;=\; \underline{w}_2\, \frac{1}{\beta_0}. \tag{52}$$

In order for $\varphi_0(\xi)$ and $\psi_0(\xi)$ to be the 0^{th} *degree elements of bi-orthonormal polynomial bases, it is required that*

$$\Psi^H\, W_2^H\, W_1\, \Phi_0 \;=\; \begin{bmatrix}1 & 0_{1,m-1}\end{bmatrix}^T,$$

$$\Phi^H\, W_1^H\, W_2\, \Psi_0 \;=\; \begin{bmatrix}1 & 0_{1,m-1}\end{bmatrix}^T,$$

cf. (42)*. By inserting* (51)–(52)*, these requirements can equivalently be written as* (49)–(50)*, which completes the proof.* ■

Note that together, (49)–(50) enable an initialization of the polynomials $\varphi_0(\xi)$ and $\psi_0(\xi)$ in terms of the weights w_{1k}, w_{2k}, $k = 1, \ldots, m$, that define the bi-linear form (32). In particular, to ensure that the polynomial bases are correctly initialized, i.e., the 0^{th} degree basis polynomials are bi-orthonormal with respect to (32), the following equality needs to hold:

$$\psi_0^* \varphi_0 = \frac{1}{\beta_0^*\, \gamma_0} = \frac{1}{\underline{\mathrm{w}}_2^H\, \underline{\mathrm{w}}_1}.$$

To support this claim, observe that, first using (47) and second using (49)–(50),

$$\begin{aligned}\Big((\Phi^H\, W_1^H)\, \underline{\mathrm{w}}_2\Big)^H \Big((\Psi^H\, W_2^H)\, \underline{\mathrm{w}}_1\Big) \\ &= \underline{\mathrm{w}}_2^H\, (W_1\, \Phi)\, (W_1\, \Phi)^{-1}\, \underline{\mathrm{w}}_1 \;=\; \underline{\mathrm{w}}_2^H\, \underline{\mathrm{w}}_1. \\ &= \begin{bmatrix}\beta_0^* & 0_{1,m-1}\end{bmatrix} \begin{bmatrix}\gamma_0 & 0_{1,m-1}\end{bmatrix}^T = \beta_0^*\, \gamma_0\,.\end{aligned}$$

In the next section, an algorithm for the derivation of the polynomial recursion coefficients for bi-orthonormal polynomial bases $\varphi_j(\xi)$ and $\psi_j(\xi)$ is presented.

5.5. An algorithm for the derivation of recurrence coefficients

In this section, it is shown how to generate the recurrence coefficients for the bi-orthonormal polynomial bases from the data that defines the bi-linear form (32). The following algorithm combines the initialization of the polynomial bases in (49)–(50) with the eigenvalue decompositions in (45)–(46).

Algorithm 22. *Let X be given in* (39)*, and $\underline{w}_1$, $\underline{w}_2$ be given in* (40)–(41)*. Then, form initial node-weight matrices $\left[\begin{array}{c|c} \underline{w}_1 & X \end{array}\right]$ and $\left[\begin{array}{c|c} \underline{w}_2 & X \end{array}\right]$. Next, compute matrices*

$$\tilde{K},\, \tilde{L} \;\in\; \mathbb{C}^{m\times m}, \qquad \tilde{L} \;=\; \tilde{K}^{-H}, \tag{53}$$

such that

$$\tilde{L}^H \left[\begin{array}{c|c} \underline{w}_1 & X \end{array}\right] \begin{bmatrix}1 & \\ & \tilde{K}\end{bmatrix} \;=\; \left[\begin{array}{c|c} \gamma_0 & \\ 0_{m-1,1} & H_1 \end{array}\right], \tag{54}$$

$$\tilde{K}^H \left[\begin{array}{c|c} \underline{w}_2 & X \end{array}\right] \begin{bmatrix}1 & \\ & \tilde{L}\end{bmatrix} \;=\; \left[\begin{array}{c|c} \beta_0 & \\ 0_{m-1,1} & H_2 \end{array}\right], \tag{55}$$

where H_1 and H_2 are upper Hessenberg matrices as in (37)–(38)*.*

A numerically reliable and efficient implementation of Alg. 22 can be obtained by exploiting elementary zeroing operations such as Givens reflections or rotations, while following the 'chasing down the diagonal' strategy in Rutishauser (1963). This approach indeed yields good results on actual data, as will be further demonstrated in Sect. 6, and is also applied in, e.g., Reichel et al. (1991), Van Barel & Bultheel (1995), Faßbender (1997).

5.6. Proving bi-orthonormality of the resulting polynomials

In this section, it is shown that the Hessenberg matrices obtained in Alg. 22 indeed contain the recurrence coefficients that generate bi-orthonormal polynomials with respect to (32). First, it is proven that the individual columns of $\tilde{K}, \tilde{L}$ in (53), viz.

$$\tilde{K} = \begin{bmatrix}\tilde{k}_1 & \tilde{k}_2 & \cdots & \tilde{k}_m\end{bmatrix},$$

$$\tilde{L} = \begin{bmatrix}\tilde{\ell}_1 & \tilde{\ell}_2 & \cdots & \tilde{\ell}_m\end{bmatrix},$$

where $\tilde{k}_j, \tilde{\ell}_j \in \mathbb{C}^{m\times 1}$, $j = 1, 2, \ldots, m$, satisfy recurrence relations.

Lemma 23. *Let $\tilde{K}, \tilde{L} \in \mathbb{C}^{m\times m}$ be such that $\tilde{L} = \tilde{K}^{-H}$ and* (54) *and* (55) *hold. In addition, let H_1 and H_2 be defined in* (37)–(38)*. Then, the columns of $\tilde{K}, \tilde{L}$ satisfy the recurrence relations*

$$X\, \tilde{k}_j \;=\; \tilde{k}_1\, \sigma_{0,j-1} \;+\; \tilde{k}_2\, \sigma_{1,j-1} \;+\; \cdots \;+\; \tilde{k}_{j+1}\, \sigma_{j,j-1}\,, \tag{56}$$

$$X\, \tilde{\ell}_j \;=\; \tilde{\ell}_1\, \tau_{0,j-1} \;+\; \tilde{\ell}_2\, \tau_{1,j-1} \;+\; \cdots \;+\; \tilde{\ell}_{j+1}\, \tau_{j,j-1}\,, \tag{57}$$

which are initialized by (see also Thm. 21)

$$\tilde{k}_1 \;=\; \underline{w}_1\, \frac{1}{\gamma_0}, \qquad \tilde{\ell}_1 \;=\; \underline{w}_2\, \frac{1}{\beta_0}. \tag{58}$$

Proof*: From the first column of* (54) *and* (55)*, it follows that*

$$\tilde{L}^H\, \underline{w}_1 \;=\; \begin{bmatrix}\gamma_0 & 0_{1,m-1}\end{bmatrix}^T \quad\Longrightarrow\quad \underline{w}_1 \;=\; \tilde{K} \begin{bmatrix}\gamma_0 & 0_{1,m-1}\end{bmatrix}^T,$$

$$\tilde{K}^H \underline{w}_2 \;=\; \begin{bmatrix}\beta_0 & 0_{1,m-1}\end{bmatrix}^T \quad\Longrightarrow\quad \underline{w}_2 \;=\; \tilde{L}\begin{bmatrix}\beta_0 & 0_{1,m-1}\end{bmatrix}^T,$$

where (53) *is used. Indeed,* (58) *follows. Next, observe that*

$$\begin{aligned} X\tilde{K} &= \tilde{K} H_1, \\ X\tilde{L} &= \tilde{L} H_2, \end{aligned}$$

by virtue of (53)*. Evaluating the* j^{th} *column of these equations,* $j = 1, 2, \ldots, m-1$*, yields* (56) *and* (57)*.* ■

Next, the recurrence coefficients in H_1 and H_2 are used to generate polynomial bases. The following result proves bi-orthonormality with respect to (32) by connecting the individual polynomials to the individual columns of $\tilde{K}$ and $\tilde{L}$.

Theorem 24. *Consider the Hessenberg decompositions* (54) *and* (55)*. Let* $\varphi_0(\xi)$ *and* $\psi_0(\xi)$ *be selected according to* (48)*. Then, the recurrence relations*

$$\begin{aligned} \varphi_j(\xi) = \frac{1}{\sigma_{j,j-1}} \Big(&(\xi - \sigma_{j-1,j-1})\,\varphi_{j-1}(\xi) \;-\; \sigma_{j-2,j-1}\,\varphi_{j-2}(\xi) \\ &-\; \cdots \;-\; \sigma_{1,j-1}\,\varphi_1(\xi) \;-\; \sigma_{0,j-1}\,\varphi_0(\xi)\Big) \end{aligned} \tag{59}$$

$$\begin{aligned} \psi_j(\xi) = \frac{1}{\tau_{j,j-1}} \Big(&(\xi - \tau_{j-1,j-1})\,\psi_{j-1}(\xi) \;-\; \tau_{j-2,j-1}\,\psi_{j-2}(\xi) \\ &-\; \cdots \;-\; \tau_{1,j-1}\,\psi_1(\xi) \;-\; \tau_{0,j-1}\,\psi_0(\xi)\Big) \end{aligned} \tag{60}$$

generate bi-orthonormal bases with respect to (32)*.*

Proof*: Combining* (51)*,* (52)*, and* (58) *yields*

$$\begin{aligned} \tilde{k}_1 &= W_1 \Phi_0, \\ \tilde{\ell}_1 &= W_2 \Psi_0. \end{aligned}$$

Then, by rewriting (59)–(60) *in the equivalent form* (33)–(34)*, if follows from* (56)–(57) *that*

$$\begin{aligned} \tilde{k}_j &= W_1 \Phi_{j-1}, \\ \tilde{\ell}_j &= W_2 \Psi_{j-1}, \end{aligned}$$

$j = 1, 2, \ldots, m$*. Hence, since*

$$\tilde{L}^H \tilde{K} \;=\; \Psi^H W_2^H W_1 \Phi \;=\; I_m,$$

bi-orthonormality of $\varphi_j(\xi)$ *and* $\psi_j(\xi)$ *follows immediately from bi-orthonormality of* $\tilde{K}$ *and* $\tilde{L}$*.* ■

To summarize, the construction of bi-orthonormal polynomial bases requires the solution of the Hessenberg decomposition of two initial node-weight matrices, see Alg. 22. Hereafter, the polynomial bases are generated using the recurrence relations in Thm. 24.

5.7. Frequency points on the imaginary axis

In the special situation where all frequency points ξ_k, $k = 1, \ldots, m$, are taken on the imaginary axis, a useful relation exists between the Hessenberg matrices H_1 and H_2 in (37)–(38).

Theorem 25. *Let* $\xi_k = \jmath\omega_k$*,* $\omega_k \in \mathbb{R}$*,* $k = 1, \ldots, m$*. Then,* H_1 *and* H_2 *are tri-diagonal matrices. Furthermore,*

$$H_1^H = -H_2.$$

Proof*: Since all frequency points are on the imaginary axis,*

$$X^H = -X,$$

see (39)*. Using* (45) *and* (46)*, it then holds that*

$$\begin{aligned} H_1^H = \Big((\Psi^H W_2^H)\, X\, (W_1 \Phi)\Big)^H \;&=\; (\Phi^H W_1^H)\, X^H\, (W_2 \Psi) \\ &= -\,(\Phi^H W_1^H)\, X\, (W_2 \Psi) = -H_2. \end{aligned}$$

This implies that H_1 *and* H_2 *are both upper and lower Hessenberg, hence, tri-diagonal matrices.* ■

By virtue of Thm. 25, *three-term-recurrence* relations can be derived in line with Thm. 24 that generate bi-orthonormal polynomial bases $\varphi_j(\xi)$ and $\psi_j(\xi)$.

5.8. Constructing bi-orthonormal 2×2 *real block-polynomials*

In Sect. 5.1–Sect. 5.7, the principle steps in the construction of bi-orthonormal polynomials have been presented. In this section, these concepts are generalized towards bi-orthonormal 2×2 real block-polynomials, which is needed to achieve optimal conditioning of Alg. II in Sect. 2.

For the identification of a real-rational transfer function $\hat{P}(\xi, \theta)$, cf. (2), the derivation of *real* polynomial recurrence coefficients is required. To this end, the property

$$\hat{P}(\xi^*, \theta) \;=\; \hat{P}^*(\xi, \theta),$$

which is characteristic for real-rational transfer functions, is exploited. Specifically, *complex-conjugate* node and weight pairs are taken in Alg. 22. This leads to the initial node-weight matrix

$$\mathcal{I}_{\text{nw}} := \left[\begin{array}{c|ccccccc} & w_{21}^H & w_{21}^T & w_{22}^H & w_{22}^T & \cdots & w_{2m}^H & w_{2m}^T \\ \hline w_{11} & \xi_1 & & & & & & \\ w_{11}^* & & \xi_1^* & & & & & \\ w_{12} & & & \xi_2 & & & & \\ w_{12}^* & & & & \xi_2^* & & & \\ \vdots & & & & & \ddots & & \\ w_{1m} & & & & & & \xi_m & \\ w_{1m}^* & & & & & & & \xi_m^* \end{array}\right], \tag{61}$$

where $w_{1k}, w_{2k} \in \mathbb{C}^{1\times 2}$, $k = 1, \ldots, m$, are given in (8) and (18). This matrix is then transformed under similarity into the matrix

$$\tilde{\mathcal{I}}_{\text{nw}} \;=\; T_0^H\, \mathcal{I}_{\text{nw}}\, T_0,$$

where

$$T_0 \;=\; \begin{bmatrix} I_2 & \\ & I_m \otimes \begin{bmatrix} 1 & \jmath \\ 1 & -\jmath \end{bmatrix} \end{bmatrix}, \qquad \jmath = \sqrt{-1}.$$

Importantly, $\tilde{\mathcal{I}}_{\text{nw}}$ is a real-valued matrix. Note that considering conjugate node and weight pairs does not lead to an increase of

complexity, since all remaining algorithmic computations can now be performed on real matrices.

Next, frequency points $\xi_k = \jmath\omega_k$, $\omega_k \in \mathbb{R}$, are considered. In line with the result in Thm. 25, the real initial node-weight matrix $\tilde{\mathcal{I}}_{\rm nw}$ is transformed into a 2×2 real block-tridiagonal matrix

$$\mathcal{T} := \left[\begin{array}{c|cccccc} & B_0^T & & & & & \\ \hline \Gamma_0 & A_1 & B_1^T & & & & \\ & \Gamma_1 & A_2 & B_2^T & & & \\ & & \Gamma_2 & \ddots & \ddots & & \\ & & & \ddots & & B_{m-1}^T & \\ & & & & \Gamma_{m-1} & A_m \end{array}\right] \tag{62}$$

under similarity. Here, the blocks $A_i \in \mathbb{R}^{2\times 2}$, $i = 1, \ldots, m$, are full matrices, whereas the blocks $B_j, \Gamma_j \in \mathbb{R}^{2\times 2}$, $j = 0, 1, \ldots, m-1$, are upper triangular matrices.

The block-tridiagonal matrix provides the recurrence coefficients that generate block-polynomials that are bi-orthonormal with respect to (30).

Theorem 26. *Consider the initial node-weight matrix $\mathcal{I}_{\rm nw}$ in* (61)*, where ξ_k, w_{1k}, w_{2k}, $k = 1, \ldots, m$, define the bi-linear form* (30)*. Let $\mathcal{I}_{\rm nw}$ be transformed under similarity into the real block-tridiagonal matrix $\mathcal{T}$ in* (62)*. Then, bi-orthonormal polynomials $\varphi_j(\xi), \psi_j(\xi) \in \mathbb{R}^{2\times 2}[\xi]$, $j = 0, 1, \ldots, n-1$, with respect to the bi-linear form* (30) *are obtained from the three-term-recurrence relations*

$$\varphi_j(s) = \left(\varphi_{j-1}(s)\,(\ s \cdot I_2 - A_j\,) \ - \ \varphi_{j-2}\,B_{j-1}^T\right)\Gamma_j^{-1}, \tag{63}$$

$$\psi_j(s) = \left(\psi_{j-1}(s)\,(-s \cdot I_2 - A_j^T) \ - \ \psi_{j-2}\,\Gamma_{j-1}^T\right)B_j^{-1}, \tag{64}$$

where A_j, B_j, $\Gamma_j \in \mathbb{R}^{2\times 2}$ follow from $\mathcal{T}$. The recursions are initialized with $\varphi_0(s) = \Gamma_0^{-1}$ and $\psi_0(s) = B_0^{-1}$.

Remark 27. *Consider the special situation that $W_2 = W_1$. In that case, the initial node-weight matrix can be transformed into a* symmetric *block-tridiagonal matrix under* unitary *similarity, see also Gragg & Harrod (1984), Van Barel & Bultheel (1992). This symmetric block-tridiagonal matrix, known as a block-Jacobi matrix, has $A_j^T = A_j$ and $\Gamma_j = B_j$. Consequently, it follows from the three-term-recurrence relations* (63)–(64) *that the polynomial bases $\varphi_j(s)$, $\psi_j(s)$ coincide into one single basis. This polynomial basis is orthonormal with respect to*

$$\langle\!\langle \varphi_i(\xi),\, \varphi_j(\xi) \rangle\!\rangle := \sum_{k=1}^{m} \varphi_j^H(\xi)\, w_{1k}^H\, w_{1k}\, \varphi_i(\xi_k), \tag{65}$$

which constitutes a matrix representation of the data-dependent inner product in Def. 9. This implies that the presented results cover the data-dependent inner product that enables optimal conditioning of Alg. I (SK) as a special case.

Summarizing, to construct bi-orthonormal 2×2 real block-polynomials, the initial node-weight matrix (61) needs to be transformed under similarity into the 2×2 real block-tridiagonal matrix (62), after which the bi-orthonormal bases are obtained using the three-term-recurrences in Thm. 26.

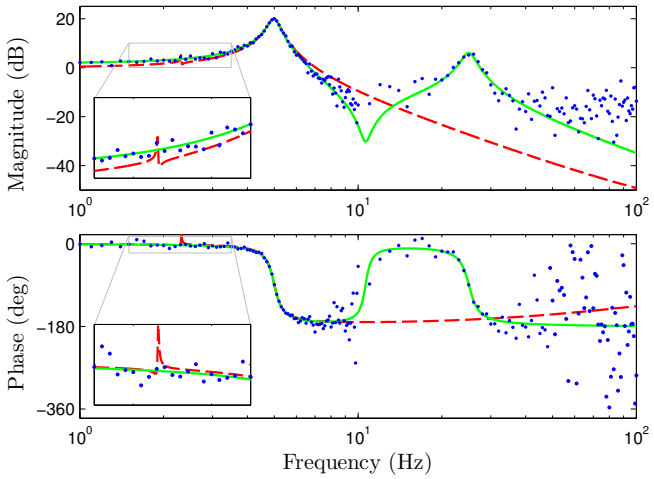

Figure 1: Noisy $m = 181$ point FRF P_o (dotted) and $n = 4^{\rm th}$ order parametric models $\hat{P}(s)$ obtained with Alg. I (SK) (dashed) and Alg. II (IV) (solid).

In the next section, the benefits of these polynomials in frequency-domain system identification algorithms are demonstrated by means of experimental examples.

6. Comparison of algorithms for identification examples

In this section, the convergence properties and numerical properties of Alg. I and Alg. II are compared for two identification examples. This constitutes Contribution C5 of the paper.

6.1. Simulation example

First, a comparison between Alg. I and Alg. II is made for a relatively simple simulation example. This enables reliable computations in both algorithms irrespective of the polynomial basis that is used, because numerical ill-conditioning is not excessive for this example and sufficiently accurate model estimates can be computed. In particular, measurements $P_o(s_k)$, $s_k = 1, \ldots, m$, are generated by contaminating the frequency response of a $4^{\rm th}$ order system, representing a typical collocated motion system, with circularly complex distributed random noise having a uniform amplitude distribution over all frequencies. Figure 1 show the resulting measurement data. It is aimed to minimize $V(\theta) = \sum_{k=1}^{m} |P_o(s_k) - \hat{P}(s_k)|^2$.

In Table 1, the converged results of Alg. I and Alg. II are shown. Again, it is emphasized that due to the simplicity of the considered example, the polynomial basis that is selected does not significantly influence the outcome of the algorithms. The results in Table 1 confirm the theoretical analysis in Whitfield (1987), i.e., the fixed point of Alg. I is not a (local) minimum of $\mathcal{V}(\theta)$, since $\left\| \frac{\partial V(\theta)}{\partial \theta^T}\Big|_{\theta=\theta_{\rm SK}^\star} \right\|_2 > 0$. In contrast, the fixed point of Alg. II corresponds to an optimum of $\mathcal{V}(\theta)$, since the first order optimality condition holds, i.e., $\left\| \frac{\partial V(\theta)}{\partial \theta^T}\Big|_{\theta=\theta_{\rm IV}^\star} \right\|_2 \approx 0$. In accordance with this result, Alg. II yields a smaller criterion value than Alg. I, i.e., $V(\theta_{\rm IV}^\star) < V(\theta_{\rm SK}^\star)$, see also Fig. 2. In fact, whereas the SK-algorithm yields a biased estimate due to the noise effects that are present in the data, the IV-algorithm

Table 1: Convergence behavior and numerical conditioning for the SK-algorithm and the IV-algorithm.

Alg.	basis	κ	$V(\theta^\star)$	$\left\| \frac{\partial V(\theta)}{\partial \theta^T}\big\|_{\theta=\theta^\star} \right\|_2$
I (SK)	φ_{mon}	$1.010 \cdot 10^6$	27.915	0.229
I (SK)	φ_{OP}	1.000	27.915	0.229
II (IV)	φ_{mon}	$5.669 \cdot 10^{15}$	6.003	$5.588 \cdot 10^{-13}$
II (IV)	$\varphi_{\text{BP}}, \psi_{\text{BP}}$	1.000	6.003	$5.588 \cdot 10^{-13}$

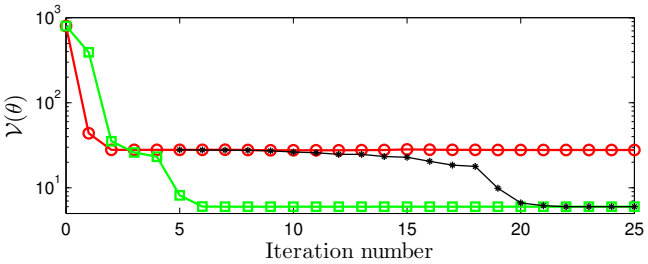

Figure 2: Convergence behavior of the SK-algorithm (○ − ○), the IV-algorithm (□ − □), and the GN-algorithm started after 5 SK-iterations (⋆ − ⋆).

successfully captures all relevant dynamical behavior of the underlying 4$^{\text{th}}$ order system, as is shown in Fig. 1.

Remark 28. *To ensure convergence to a (local) optimum, it is common to apply a gradient-based search after convergence of the SK-algorithm. In particular, the SK-algorithm is commonly used to initialize (damped) Gauss-Newton (GN) iterations, see, e.g., Bayard (1994). Indeed, in the considered example, the same minimum of the cost function as obtained using the IV-algorithm can also be obtained by means of GN-iterations, initialized with the SK-algorithm. However, this goes at the expense of a significant increase of the number of required iterations, hence, a larger computation time, see Fig. 2.*

Next, the numerical properties associated with both frequency-domain identification algorithms are investigated. When the monomial basis, see Example 2, is used in Alg. I, then the maximum condition number during the iterations is $\kappa(W_1\,\Phi) = 1.010 \cdot 10^6$. For Alg. II, the maximum condition numbers are approximately quadratically larger, confirming Cor. 7. For this example, it even holds that $\kappa(\Psi^H\,W_2^H\,W_1\,\Phi) > \kappa(W_1\,\Phi)^2 = 5.669 \cdot 10^{15}$.

The results in this paper enable a numerically reliable implementation of both frequency-domain identification algorithms. Importantly, by using two sets of *bi-orthonormal polynomials* with respect to the bi-linear form (30), optimal numerical conditioning of Alg. II is achieved, i.e., $\kappa(\Psi^H\,W_2^H\,W_1\,\Phi) = 1$. In the special case where $W_2 = W_1$, the bi-orthonormal polynomials introduced in this paper coincide into a single set of *orthonormal polynomials* with respect to the data-dependent inner product (65). Indeed, such polynomial basis leads to optimal conditioning in Alg. I, i.e., $\kappa(W_1\,\Phi) = 1$, see also Bultheel et al. (2005). It is emphasized that the key new aspect in this paper is the combination of the enhanced convergence properties of Alg. II with optimal numerical conditioning in frequency-domain identification.

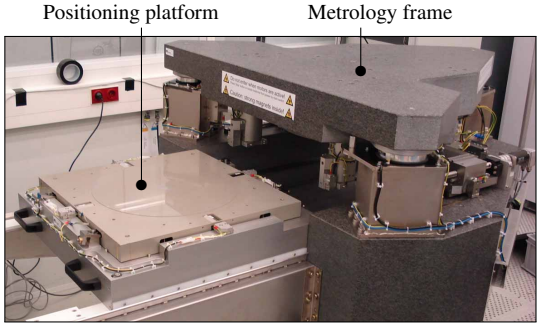

Figure 3: Lightweight positioning platform used in IC manufacturing machines.

6.2. *Experimental example*

In this section, the frequency-domain identification algorithm that is proposed in this paper is applied to an industrial motion system. In particular, the prototype wafer stage in Fig. 3 is considered. A wafer stage is part of lithographic IC manufacturing devices, used to position ICs with respect to a light source. Market viability of IC manufacturing devices requires nanometer positioning accuracy as well as a high throughput. Since a high throughput demands large accelerations, next-generation wafer stages are designed to be lightweight. However, as a consequence, these stages tend to show structural deformations, which obstruct the desired positioning accuracy. Typically, such deformations manifest in all degrees of freedom of the wafer stage. Therefore, multivariable, model-based control design is indispensable to achieve high positioning accuracy, see also Oomen et al. (2014). A corner stone for successful multivariable control design is a reliable algorithm for parametric identification, which captures all relevant flexible dynamical behavior of the system with high accuracy.

The wafer stage in Fig. 3 is operated contactless on the basis of magnetic levitation. As a consequence, there are six motion degrees of freedom (DOFs) of the system, viz. three translations and three rotations. In this paper, the behavior of the wafer stage for vertical translations is investigated. In particular, the relation between forces F_z $[N]$ that are applied in the vertical direction and resulting displacements z $[m]$ in the vertical direction is considered. Figure 4 shows a frequency response function (FRF) identification $P_o(s_k)$, $s_k = \jmath \cdot 2\pi \cdot [1, 3, \ldots, 2449]$ rad/s.

Next, a 16$^{\text{th}}$ order parametric transfer function model $\hat{P}(s)$ of the system's behavior is estimated. A maximum likelihood criterion is considered, see Pintelon & Schoukens (1990), (Pintelon & Schoukens, 2001, Chap. 7), and (McKelvey, 2002, Sect. 3). To this end, (1) is minimized with $W(s_k) = 1 \,/\, \sigma_{P_o}(s_k)$, where $\sigma^2_{P_o}(s_k)$ is the variance on the non-parametric FRF data as shown in Fig. 4. Hence,

$$\mathcal{V}_{\text{ML}}(\theta) := \sum_{k=1}^{m} \left| \frac{(P_o(s_k) \;-\; \hat{P}(s_k, \theta))}{\sigma_{P_o}(s_k)} \right|^2 . \qquad (66)$$

To optimize the maximum likelihood criterion (66), Alg. II is employed. During the iterations, $\kappa(\Psi^H\,W_2^H\,W_1\,\Phi) < 1.008$, i.e., the use of bi-orthonormal polynomials yields optimal numerical conditioning. This facilitates reliable, accurate

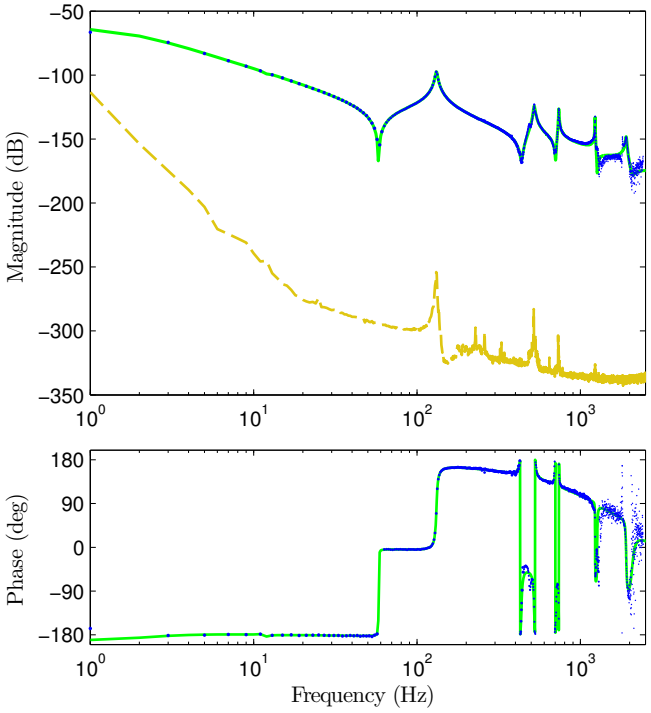

Figure 4: Measured $m = 1250$ point FRF P_o (dotted) with corresponding variance (dashed), and $n = 16^{\text{th}}$ order parametric model $\hat{P}(s)$ (solid).

computations. In contrast, when the monomial basis is used, the worst-case condition number that is observed equals $\kappa(\Phi_{\text{mon}}^H W_2^H W_1 \Phi_{\text{mon}}) = 1.181 \cdot 10^{98}$. Although for the considered identification problem it is still possible to compute an accurate model after appropriate scaling, such high condition numbers lead to a numerical breakdown for multivariable systems such as the one presented in Oomen et al. (2014), Oomen & Steinbuch (to appear).

Upon convergence of the algorithm, $V(\theta_{\text{IV}}^\star) = 1.727 \cdot 10^3$, whereas $\left\| \frac{\partial V(\theta)}{\partial \theta^T}\Big|_{\theta=\theta_{\text{IV}}^\star} \right\|_2 = 8.5831 \cdot 10^{-5} \approx 0$, i.e., a (local) minimum of the cost function is attained. Indeed, in Fig. 4 it is observed that the obtained model describes the system's behavior with high accuracy, demonstrating the effectiveness of Alg. II for frequency-domain system identification.

7. Conclusions

In this paper, a new algorithm for frequency-domain system identification is presented that combines advantageous convergence properties in frequency-domain instrumental variable (IV) identification with computational algorithms that yield optimal numerical conditioning. The key novel technical result of this paper is the introduction of two bi-orthonormal polynomial bases with respect to a data-dependent bi-linear form in system identification. By using these bi-orthonormal bases in the IV-algorithm, viz. one polynomial basis to parameterize the to-be-estimated model and another polynomial basis to parameterize the instrument, optimal numerical conditioning is achieved. In addition, optimal conditioning for the classical SK-algorithm is retrieved as a special case, in which the two polynomial bases coincide into a single basis that is orthonormal with respect to a data-dependent inner product.

A simulation example confirms that the convergence behavior of the IV-algorithm is beneficial in frequency-domain identification. In particular, for the considered example, the SK-algorithm suffers from a bias that is induced by the noise on the measurement data. The IV-algorithm outperforms the SK-algorithm and yields an unbiased estimate. Furthermore, the IV-algorithm is successfully applied for identification of the dynamical behavior a high-precision motion system. Indeed, the use of bi-orthonormal polynomials provides optimal numerical conditioning in all iterations. Thus, the iterations are performed with high reliability, leading to an accurate parametric model of the system under study.

Although the material that is presented in this paper is concentrated on identification of single-input single-output systems, all obtained results can be generalized towards multivariable systems. For this purpose, a system representation in the form of a matrix fraction description can be employed, as is also considered in Blom & Van den Hof (2010). First results are presented in Van Herpen (2014, Chap. 4, App. A).

In practice, both Alg. I and Alg. II show convergence to a stationary point for most data sets, especially when the signal to noise ratio is sufficiently high. Indeed, both frequency-domain algorithms are widely applied for system identification (Pintelon et al., 1994). Important convergence aspects have been further studied in detail in Söderström & Stoica (1988), Regalia et al. (1997).

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