

Bi-Orthonormal Polynomial Basis Function Framework with Applications in System Identification

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Abstract—Numerical aspects are of central importance in identification and control. Many computations in these fields involve approximations using polynomial or rational functions that are obtained using orthogonal or oblique projections. The aim of this paper is to develop a new and general theoretical framework to solve a large class of relevant problems. The proposed method is built on the introduction of bi-orthonormal polynomials with respect to a data-dependent bi-linear form. This bi-linear form generalises the conventional inner product and allows for asymmetric and indefinite problems. The proposed approach is shown to lead to optimal numerical conditioning ($\kappa = 1$) in a recent frequency-domain instrumental variable system identification algorithm. In comparison, it is shown that these recent algorithms exhibit extremely poor numerical properties when solved using traditional approaches.

I. INTRODUCTION

Applications of system identification and control often involve numerical computations. The accuracy of these computations determines the quality of the resulting model or controller. This has led to considerable research to develop numerically reliable algorithms, see, e.g., [38] and [8], [4] for a general overview. Many computations involve weighted least-squares type problems for systems that are parametrized in terms of (vector) polynomials or rational forms, where orthogonal or oblique projections play a central role.

In the field of system identification, weighted nonlinear least-squares criteria are particularly common, see [29]. Established identification algorithms include [26], the SK-iteration [34], and the Gauss-Newton iteration [1], which (iteratively) compute the least-squares solution to a linear systems of equations, for polynomial models or rational parametrizations. Although conceptually straightforward, the associated numerical conditioning is often extremely poor, as is evidenced by the developments in [1], [18], [28], [41], [44], which provide partial solutions for ill-conditioning. In [30], [37], [21], a fundamentally different solution strategy is pursued. The strategy is based upon the construction of orthogonal polynomials with respect to a data-dependent inner product, which directly provides the solution to the approximation problem in terms of polynomials. Essentially, this yields optimal conditioning of the associated linear system of equations, i.e., $\kappa = 1$.

Besides developments in view of reliable algorithms that involve least-squares type solutions, recently, more general

algorithms with favorable convergence properties have been developed in, e.g., system identification. Indeed, the commonly used SK-algorithm [34] often does not converge to a minimum of the underlying nonlinear least-squares criterion, as is proved in [42]. In [3], a system identification algorithm is presented that guarantees convergence to a minimum of this criterion by introducing an algorithm that has the interpretation of an instrumental variable method [35]. From a computational perspective, the approach in [3] involves a more general polynomial approximation problem, since the algorithms in [26], [34], [1] are recovered as a special case.

Although recent generalizations of algorithms for weighted nonlinear least-squares problems have improved certain aspects, including the convergence properties in system identification algorithms, the solution strategy towards optimal conditioning by means of the orthogonal polynomial framework in [30], [37], [21] is not applicable in this general situation. In particular, in the general case, the polynomial approximation problem has an asymmetric and indefinite form. As a consequence, the idea of tailoring the inner product, which is the essential step in [30], [37], [21], cannot be applied, since a tailored inner product requires symmetry and positive-definiteness. The aim of this paper is to develop a theory that addresses the general situation by accounting for asymmetry and indefiniteness of the approximation problem. The key step taken in this paper is to replace the conventional inner product by a new bi-linear form, involving two sets of polynomials. In terms of classical algorithms, the proposed framework can be interpreted as achieving optimal conditioning ($\kappa = 1$) for the general situation.

The main contribution of this paper is the development of a new polynomial theory for solving a general class of problems that are encountered in recent algorithms in the field of identification and control, including those in time-domain identification [46], [35], [13], frequency-domain identification [3], and control [27]. In particular, it is shown that a general class of polynomial approximation problems, underlying the aforementioned applications, involves an asymmetric form. As a first contribution, it is shown that by selecting bi-orthonormal polynomial bases with respect to a data-dependent bi-linear form associated with such a polynomial approximation problem, i) the optimal approximant of a certain degree is equal to a scaled version of the right basis polynomial of corresponding degree, which has as an immediate effect that ii) the linear system of equations that results after substitution of the polynomial bases has optimal numerical conditioning. In addition, it is proved that this result cannot be obtained through the use of a single polynomial basis, as is considered in [30], [37], [21], since the latter only apply to the symmetric and positive definite case. For the construction of bi-orthonormal

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polynomial bases, the associated oblique projection in linear algebra is investigated, which is defined through two Krylov subspaces. Bi-orthonormal bases of these Krylov subspaces are shown to directly lead to the desired polynomials. Finally, the basic principle for computing these bases is demonstrated through an explicit algorithm for bi-orthonormalization on the real line. In the present paper, fundamental theory and properties of the framework are developed. Preliminary results of this research appear in [20] and [19, Chap. 2]. Further applications to specific identification problems are developed in [19, Chap. 3], [22], where a vector polynomial framework is employed.

This paper is organized as follows. In Sect. II, the polynomial approximation problem and corresponding linear algebra formulation associated with the algorithm in [3] is given, which includes the conventional polynomial approximation problem associated with the algorithm in [34] as special case. The main result of this paper is given in Sect. IV, which explains the role of bi-orthonormal polynomials in the computation of accurate solutions to the general polynomial approximation problem. In Sect. V, it is shown that bi-orthonormal polynomials can be constructed efficiently using three-term-recurrence relations. In Sect. VI, an algorithm to construct real-valued bi-orthonormal polynomials is provided. In Sect. VII, an example is given that confirms optimal numerical conditioning for the general class of polynomial approximation problems. Conclusions are drawn in Sect. VIII. Finally, all proofs are presented in Appendix B.

Implementation guideline. Readers interested in directly applying the approach in this paper are suggested to formulate the problem in terms of (1). Next, compute the tridiagonal matrix in (45) using Algorithm 39. Then, compute bi-orthonormal bases using the three-term-recurrence relations in (48)–(49). Finally, the desired solution immediately follows from (24).

II. POLYNOMIAL APPROXIMATION: APPLICATIONS IN IDENTIFICATION AND CONTROL

A. Problem formulation

The aim of this paper is to determine the solution $f(\xi, \theta)$ to a type of polynomial equality of the form

$$\sum_{k=1}^m \frac{\partial g(\xi_k, \theta)}{\partial \theta^T} w_{2k}^H w_{1k} f(\xi_k, \theta) = 0. \quad (1)$$

where $w_{1k}, w_{2k} \in \mathbb{C}^{1 \times q}$ are the weights specified by the problem at hand. Furthermore, $f(\xi, \theta), g(\xi, \theta) \in \mathbb{C}^{q \times 1}[\xi]$ are q -dimensional vector-polynomials:

$$f(\xi, \theta) = \sum_{j=0}^n \varphi_j(\xi) \theta_j, \quad (2)$$

$$g(\xi, \theta) = \sum_{j=0}^{n-1} \psi_j(\xi) \theta_j, \quad (3)$$

where $\varphi_j(\xi), \psi_j(\xi) \in \mathbb{C}^{q \times q}[\xi]$ are q -dimensional block-polynomials in the variable $\xi \in \mathbb{C}$ with nodes $\xi_k, k = 1, \dots, m$. Furthermore, $\theta_j \in \mathbb{C}^{q \times 1}, j = 0, 1, \dots, n$ are parameter vectors.

An example of a commonly used block-polynomial basis is the monomial basis

$$\phi_{\text{mon},j}(\xi) = \xi^j I_q. \quad (4)$$

In this paper, this monomial basis is used for comparison, as more general choices for $\varphi(\xi)$ and $\psi(\xi)$ are proposed. Note that it is immediate to express general block-polynomials $\varphi_j(\xi), \psi_j(\xi)$ in terms of $\phi_{\text{mon},i}(\xi), i = 0, 1, \dots, j$.

The following assumptions are imposed throughout to facilitate the presentation.

Assumption 1. *The nodes $\xi_k, k = 1, \dots, m$, are distinct.*

Assumption 2. *The weights $w_{1k}, w_{2k}, k = 1, \dots, m$, are non-zero.*

Note that in the presence of weights that are equal to zero, (1) can be reformulated as an equivalent sum of non-zero elements representing a smaller set of nodes.

Assumption 3. *The degree n of the vector polynomial $f(\xi, \theta)$ that forms the solution to (1) is assumed to be smaller than the number of nodes m .*

Assumption 4. *Both $\varphi_j(\xi)$ and $\psi_j(\xi)$ are of strict degree j , with upper triangular leading coefficient matrix, i.e.,*

$$\varphi_j(\xi) = \xi^j s_{jj} + \dots + \xi s_{j1} + s_{j0}, \quad (5)$$

$$\psi_j(\xi) = \xi^j t_{jj} + \dots + \xi t_{j1} + t_{j0}, \quad (6)$$

$s_{j0}, s_{j1}, \dots, s_{jj}, t_{j0}, t_{j1}, \dots, t_{jj} \in \mathbb{C}^{q \times q}$, where s_{jj}, t_{jj} are non-singular upper triangular matrices.

Assumption 5. *Given certain polynomial bases $\varphi_j(\xi), \psi_j(\xi)$, the parameter vectors $\theta_j \in \mathbb{C}^{q \times 1}, j = 0, 1, \dots, n$ in (2)–(3) form the variable θ in (1) that is to be determined. To avoid the trivial solution $\theta = 0$, additional constraints need to be imposed. A common solution is to enforce a subset of polynomials to be monic [9]. In the notation of this paper, this amounts to*

$$\theta_n = s_{nn}^{-1} [\underbrace{1 \dots 1}_{q_1} \underbrace{0 \dots 0}_{q_2}]^T, \quad (7)$$

where $q = q_1 + q_2$, the sum in (2) reduces to

$$f(\xi, \theta) = \sum_{j=0}^{n-1} \varphi_j(\xi) \theta_j + f_n(\xi), \quad (8)$$

with pre-determined vector-polynomial

$$f_n(\xi) := \varphi_n(\xi) \theta_n = [\underbrace{\xi^n \dots \xi^n}_{q_1} \underbrace{0 \dots 0}_{q_2}]^T + \quad (9)$$

$$\sum_{i=0}^{n-1} \xi^i s_{ni} s_{nn}^{-1} [\underbrace{1 \dots 1}_{q_1} \underbrace{0 \dots 0}_{q_2}]^T.$$

Generalization to other constraints follows similarly.

B. Applications in system identification and control

The class of polynomial approximation problems (1) is commonly encountered in system identification and control. Indeed, in frequency-domain identification, see [29], the form (1) is directly obtained in case the recent algorithm in [3] is used, as is shown in Appendix A, Alg. 43. Furthermore, (1) is inherently connected with instrumental variables (IV) identification, see [46], [35], [13]. Essentially, the parameters θ of a model identified by IV methods follow from solving a system of equations of the form

$$\sum_{t=1}^m \zeta(t)\epsilon(t, \theta) = \underline{\zeta}^T \underline{\epsilon}(\theta) = 0.$$

This system of equations can be reformulated equivalently in the frequency-domain as

$$\underline{\zeta}^T \mathcal{F}^H \mathcal{F} \underline{\epsilon}(\theta) = \underline{Z}^T \underline{E}(\theta) = \sum_{k=1}^m Z(z_k) E(z_k, \theta) = 0, \quad (10)$$

by virtue of the fact that the Discrete Fourier Transform matrix

$$\mathcal{F} := \frac{1}{\sqrt{m}} \begin{bmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & \omega_m & \omega_m^2 & \dots & \omega_m^{m-1} \\ 1 & \omega_m^2 & \omega_m^4 & \dots & \omega_m^{2(m-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \omega_m^{m-1} & \omega_m^{2(m-1)} & \dots & \omega_m^{(m-1)(m-1)} \end{bmatrix},$$

$\omega_m := e^{-j\frac{2\pi}{m}}$, is a unitary matrix. The equivalent frequency-domain formulation (10) of IV-methods is of the form (1). Finally, the form (1) is encountered in some control design approaches, such as iterative controller tuning based on correlations [27].

Note that the general form (1) encompasses many problems involving a standard least-squares problem, as is formalized in the following remark.

Remark 6. A special case of (1) is the conventional least-squares polynomial approximation problem

$$\min_{\theta} \|w_1 f(\xi, \theta)\|_2^2, \quad (11)$$

where

$$\|w_1 f(\xi, \theta)\|_2^2 := \sum_{k=1}^m f(\xi_k, \theta)^H w_{1k}^H w_{1k} f(\xi_k, \theta).$$

The first order necessary and sufficient condition for optimality in (11) reads

$$\sum_{k=1}^m \frac{\partial f(\xi_k, \theta)}{\partial \theta^T} w_{1k}^H w_{1k} f(\xi_k, \theta) = 0. \quad (12)$$

As before, the degree constraint (7) is imposed, i.e., (8) holds. Then, (12) is a special case of (1), where $\psi_j(\xi) = \varphi_j(\xi)$, $j = 0, 1, \dots, n-1$ and $w_{2k} = w_{1k}$, $k = 1, \dots, m$.

Least-squares polynomial approximation (11) is used in frequently applied identification algorithms such as [26] and the SK-iteration [34]. The connection between these algorithms and (11) is further established in Appendix A, Alg. 44. In addition, similar connections to the Gauss-Newton iteration,

see [1], exist. In this paper, the general polynomial approximation problem (1) is considered, which encompasses (11) as a special case.

As a final comment, it is often desired in both identification and control to work with models that have real-valued parameters. This can be directly enforced, as is shown in the following remark for frequency-domain approximation problems.

Remark 7. Note that the partial derivative in (1) should be interpreted as in [29, Appendix 7.X], since θ is complex-valued. On the other hand, in common frequency-domain polynomial approximation problems, nodes are selected on the imaginary axis, i.e., $\xi_k = j\omega_k$, $\omega_k \in (0, \infty)$, or on the unit circle, i.e., $\xi_k = e^{j\theta_k}$, $\theta_k \in (0, \pi)$. Many systems have real-valued coefficients, hence a real-valued solution $f(\xi, \theta) \in \mathbb{R}^{q \times q}[\xi]$ to (1) is desired. To that end, real-valued basis polynomials $\varphi_j(\xi), \psi_j(\xi) \in \mathbb{R}^{q \times q}[\xi]$ should be selected. Furthermore, (1) should then be formulated in terms of complex-conjugate nodes and weights, i.e., $\xi_k = \xi_{(k-1)}^*$ and $w_{1k} = w_{1(k-1)}^*$, $w_{2k} = w_{2(k-1)}^*$, $k = 2, 4, \dots, m$. Then, (1) can be directly recast as a real-valued problem, see also [29, Sect. 13.8], in which case the results in this paper yield $\theta_j \in \mathbb{R}^{q \times 1}$, $j = 0, 1, \dots, n$, and hence $f(\xi, \theta) \in \mathbb{R}^{q \times q}[\xi]$.

III. NUMERICAL CONDITIONING OF POLYNOMIAL APPROXIMATION PROBLEMS

A commonly pursued approach to solve the polynomial approximation problem (11) and (1) is to

- 1) Select basis polynomials φ, ψ .
- 2) Formulate and solve as a linear algebra problem.

In this section, this solution approach is investigated, as it provides a means to assess the associated numerical conditioning. It is emphasized that the main contribution of this paper lies in selecting a certain polynomial basis in Step 1, that renders superfluous Step 2 or equivalently leads to a linear systems of equations with condition number 1.

A. Reformulation as a linear algebra problem

If $\varphi_j(\xi)$ and $\psi_j(\xi)$ are pre-selected, then (1) is equivalent to the linear system of equations

$$(\Psi^H W_2^H W_1 \Phi) \theta = -\Psi^H W_2^H W_1 \Phi_n \theta_n, \quad (13)$$

with polynomial matrices

$$\Phi = \begin{bmatrix} \varphi_0(\xi_1) & \varphi_1(\xi_1) & \dots & \varphi_{n-1}(\xi_1) \\ \varphi_0(\xi_2) & \varphi_1(\xi_2) & \dots & \varphi_{n-1}(\xi_2) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_0(\xi_m) & \varphi_1(\xi_m) & \dots & \varphi_{n-1}(\xi_m) \end{bmatrix}, \quad \Phi_n = \begin{bmatrix} \varphi_n(\xi_1) \\ \varphi_n(\xi_2) \\ \vdots \\ \varphi_n(\xi_m) \end{bmatrix}, \quad (14)$$

$$\Psi = \begin{bmatrix} \psi_0(\xi_1) & \psi_1(\xi_1) & \dots & \psi_{n-1}(\xi_1) \\ \psi_0(\xi_2) & \psi_1(\xi_2) & \dots & \psi_{n-1}(\xi_2) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_0(\xi_m) & \psi_1(\xi_m) & \dots & \psi_{n-1}(\xi_m) \end{bmatrix}, \quad (15)$$

parameter vector $\theta = [\theta_0^T \ \theta_1^T \ \dots \ \theta_{n-1}^T]^T$, and weight matrices

$$W_1 = \begin{bmatrix} w_{11} & & & \\ & w_{12} & & \\ & & \ddots & \\ & & & w_{1m} \end{bmatrix}, \quad W_2 = \begin{bmatrix} w_{21} & & & \\ & w_{22} & & \\ & & \ddots & \\ & & & w_{2m} \end{bmatrix}. \quad (16)$$

Here, $\Phi, \Psi \in \mathbb{C}^{mq \times nq}$, $\Phi_n \in \mathbb{C}^{mq \times q}$, $\theta \in \mathbb{C}^{nq \times 1}$, and $W_1, W_2 \in \mathbb{C}^{m \times mq}$. Note that θ_n is a result of (7).

Assumption 8. In (13), $\Psi^H W_2^H W_1 \Phi$ is assumed to be a regular matrix.

Assumption 8 is non-restrictive. Essentially, it guarantees that a unique solution to (1) exists. Clearly, this depends on w_{1k}, w_{2k} and the selected degree n of the polynomials $f(\xi, \theta), g(\xi, \theta)$ in the polynomial approximation problem. This aspect is well-known and is analyzed in detail in [5] for the case that $w_{2k} = w_{1k}$.

In terms of linear algebra, (13) represents an *oblique*, i.e., non-orthogonal, projection, see [33, Sect. 1.12.3, Sect. 5.2.3]. For the pre-selected $\varphi_j(\xi)$ and $\psi_j(\xi)$, (13) is a linear system of equations that can be solved for θ . The accuracy of the solution θ strongly depends on the numerical conditioning of the system of equations. In Sect. III-B, it is shown that this conditioning can be extremely poor for commonly used basis functions.

Before proceeding to the numerical properties, the special case in Remark 6 is investigated.

Remark 9. For the special case in Remark 6, (12) can be written as an orthogonal projection

$$(\Phi^H W_1^H W_1 \Phi) \theta = -\Phi^H W_1^H W_1 \Phi_n \theta_n. \quad (17)$$

Hence, (17) also is recovered as a special case of (13) by setting $\Psi = \Phi$ and $W_2 = W_1$.

B. Numerical accuracy of the solution

The accuracy of the solution of (13) and (17) depends on the numerical accuracy. A standard approach to characterize the worst-case propagation of numerical round-off errors in solving (13) and (17) is the condition number, see [15, Sect. 5.3.7] for a detailed explanation. In particular, $\kappa(\Psi^H W_2^H W_1 \Phi)$ determines the accuracy of the solution θ to (13).

The weight matrices W_1 and W_2 typically follow from the problem data, e.g., the measured data in system identification. As a result, the only degree of freedom in the condition number $\kappa(\Psi^H W_2^H W_1 \Phi)$ is the choice of the polynomial bases $\varphi_j(\xi)$ and $\psi_j(\xi)$. Commonly, the monomial basis (4) is chosen, i.e.,

$$\varphi_j(\xi) = \psi_j(\xi) = \phi_{\text{mon},j}(\xi), \quad j = 0, 1, \dots, n-1.$$

In many applications, including frequency-domain system identification, this choice of basis functions typically leads to $\kappa(\Phi_{\text{mon}}^H W_2^H W_1 \Phi_{\text{mon}}) \gg 1$, i.e., a severely ill-conditioned system of equations (13). This is confirmed in real-life identification applications, where no accurate models can be obtained with standard machine precision, see [6].

Remark 10. The orthogonal projection (17) constitutes the normal equations associated with the system of equations

$$W_1 \Phi \theta = -W_1 \Phi_n \theta_n. \quad (18)$$

Instead of solving (17), it is generally preferable to determine the least-squares solution to (18) by means of a QR-factorization, see, e.g., [15, Chap. 5]. Indeed, this reduces

the sensitivity to numerical errors, since the condition number $\kappa(W_1 \Phi)$ associated with (18) is quadratically smaller than $\kappa(\Phi^H W_1^H W_1 \Phi) = \kappa(W_1 \Phi)^2$ associated with (17).

The lefthand side of the *oblique* projection (13) is not a positive definite form, in contrast to (17). Consequently, a similar approach as in Remark 10 cannot be used to enhance the conditioning of (13). Hence, the conditioning associated with (13) generally is significantly worse compared to (17)-(18), since typically $\kappa(\Psi^H W_2^H W_1 \Phi) \gg \kappa(W_1 \Phi)$. This confirms the need to develop numerically reliable solutions to (1).

In the next section, the solution strategy in this paper is outlined by showing that a careful selection of the polynomial basis that is tailored to the problem data W_1 and W_2 is essential to achieve high numerical accuracy of the solution to (17) and (13).

C. Selection of a data-dependent polynomial basis

The key observation in Sect. III-B is that the conditioning associated with (1) for pre-specified bases depends on both the problem-specific data and the selected bases. As a result, any standard polynomial basis, including monomial, Chebyshev, and Legendre basis, can potentially lead to a badly conditioned linear system of equations (13) or (17), respectively, for certain problem-specific data.

The central idea is to connect problem-specific data to the selection of the basis to enhance numerical conditioning. For the specific class of least-squares polynomial approximation problems in Remark 6 and Remark 9, a similar approach has been pursued in [6], where the problem-specific data W_1 is explicitly used in the basis. In particular, for given ξ_k and w_{1k} in (12), the inner product

$$\langle\langle \varphi_i(\xi), \varphi_j(\xi) \rangle\rangle := \sum_{k=1}^m \varphi_j(\xi_k)^H w_{1k}^H w_{1k} \varphi_i(\xi_k), \quad (19)$$

is considered, see also [10], [45]. The result (19) constitutes a generalization towards block-polynomials of a *data-dependent discrete inner product* for vector-polynomials, see also [7, Sect. 1.1–1.2] and Remark 14 in Sect. IV-B, for a further explanation. It is immediate that $\langle\langle \varphi_i(\xi), \varphi_j(\xi) \rangle\rangle$ constitutes the $q \times q$ -block-element (j, i) of the matrix $\Phi^H W_1^H W_1 \Phi$ in (17). Hence, when selecting a block-polynomial basis that is orthonormal with respect to (19), the following key results are achieved.

- i) The optimal approximant $f(\xi, \theta^*)$ to (11) immediately follows from the highest degree basis polynomial $\varphi_n(\xi)$, viz.

$$f(\xi, \theta^*) = f_n(\xi) = \varphi_n(\xi) \theta_n, \quad (20)$$

see also (9).

- ii) The associated system of equations (18) has $\kappa(W_1 \Phi) = 1$. Equivalently, $\kappa(\Phi^H W_1^H W_1 \Phi) = 1$ in (17).

For a proof of the results above, see, e.g., [5] and [30], [11]. Note that Result (i) implies that (17) or (18) need not be solved explicitly anymore.

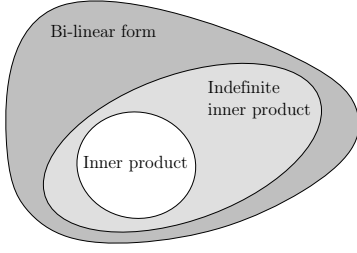


Fig. 1. Venn-diagram corresponding to Def. 11 and Lem. 13, which indicates special sub-classes of a general bi-linear form.

Note that the inner product (19) relies on symmetry and positive definiteness. As a result, it cannot be used for the general form (1). Thus, the fundamental difference of (1) compared with (12) is the lack of symmetry and positive definiteness, as is shown in detail in the forthcoming section. The key idea in this paper is a new bi-linear form that replaces (19), enabling a result for the polynomial approximation problem (1) that resembles Result (i) and (ii).

IV. BI-ORTHONORMAL BASIS POLYNOMIALS FOR SOLVING OBLIQUE PROJECTIONS

In this section, the main result of this paper is presented. First, in Sect. IV-A, a new bi-linear form is introduced that replaces the earlier considered inner product (19). Then, in Sect. IV-B, it is shown that by formulating the polynomial approximation problem (1) using two polynomial bases that are bi-orthonormal with respect to this bi-linear form, optimal numerical conditioning is achieved. Finally, in Sect. IV-C, the relation between asymmetry and bi-orthonormal polynomials is explored.

A. Relaxations of the conventional inner product

In this section, the notion of an inner product is extended towards a more general bi-linear form $[\cdot, \cdot]$ that plays a central role in the remainder of this paper. The following definition unifies related concepts in the literature.

Definition 11. Let \mathcal{V} be a vector space and let \mathbb{F} be a field of scalars. For a mapping $[\cdot, \cdot] : \mathcal{V} \times \mathcal{V} \mapsto \mathbb{F}$, consider the following four properties for all $x, y, z \in \mathcal{V}$ and all scalars $\alpha, \beta \in \mathbb{F}$.

- i) *Linearity argument 1:* $[\alpha x + \beta y, z] = \alpha[x, z] + \beta[y, z]$.
- ii) *Non-degeneracy:* if $[x, y] = 0 \forall y \in \mathcal{V}$, then $x = 0$.
- iii) *Conjugate symmetry:* $[x, y] = [y, x]^*$.
- iv) *Non-negativity:* $[x, x] \geq 0$.

Then, $[\cdot, \cdot]$ defines

- (a) an **inner product** if Prop.(i)-(ii)-(iii)-(iv) hold,
- (b) an **indefinite inner product** if Prop. (i)-(ii)-(iii) hold,
- (c) a **bi-linear form** if Prop. (i)-(ii) hold.

In this paper, the vector space \mathcal{V} in Def. 11 represents either an Euclidian space or a space of polynomials. In addition, \mathbb{F} represents either the real numbers \mathbb{R} or complex numbers \mathbb{C} .

From Def. 11, the bi-linear form includes the indefinite inner product as a special case. In turn, the indefinite inner

product includes the conventional inner product as a special case. These relations are further illustrated in Fig. 1.

Remark 12. The non-degeneracy property for inner products is often defined in a different but equivalent manner. In particular, if Prop. (iv) holds, then Prop. (ii) is equivalently given by: $[x, x] = 0 \iff x = 0$. Thus, the definition of the inner product in Def. 11 corresponds with, e.g., [24, Sect. 3.1]. Similarly, the definition of the indefinite inner product corresponds with, e.g., [14, Sect. 2.1].

In order to solve (1), its asymmetric and indefinite character is explicitly addressed, as motivated in Sect. III-C. Therefore, the following data-dependent form is introduced.

Lemma 13. Let distinct nodes $\xi_k \in \mathbb{C}$, $k = 1, \dots, m$, and corresponding weights $w_{1k}, w_{2k} \in \mathbb{C}^{1 \times q}$ be given. For vector-polynomials $\underline{\varphi}_\kappa(\xi), \underline{\psi}_\ell(\xi) \in \mathbb{C}^{q \times 1}[\xi]$, $\kappa, \ell = 0, 1, \dots, (n-1)q$, consider the data-dependent form:

$$[\underline{\varphi}_\kappa(\xi), \underline{\psi}_\ell(\xi)] := \sum_{k=1}^m \underline{\psi}_\ell(\xi_k)^H w_{2k}^H w_{1k} \underline{\varphi}_\kappa(\xi_k). \quad (21)$$

- (a) If $w_{2k} = w_{1k}$, $k = 1, \dots, m$, then $[\underline{\varphi}_\kappa(\xi), \underline{\varphi}_\ell(\xi)]$ defines a data-dependent inner product.
- (b) If $w_{2k}^H w_{1k} = w_{1k}^H w_{2k}$, $k = 1, \dots, m$, then $[\underline{\varphi}_\kappa(\xi), \underline{\varphi}_\ell(\xi)]$ defines a data-dependent indefinite inner product.
- (c) For general w_{1k}, w_{2k} , $k = 1, \dots, m$, $[\underline{\varphi}_\kappa(\xi), \underline{\psi}_\ell(\xi)]$ defines a data-dependent bi-linear form.

Proof: Follows by verifying the properties of an inner product, indefinite inner product, and bi-linear form in Def. 11. ■

Remark 14. The form $\langle\langle \varphi_i(\xi), \varphi_j(\xi) \rangle\rangle$ in (19) is a natural extension of Lemma 13-(a), which is defined for vector-polynomials, towards block-polynomials $\varphi_i(\xi) \in \mathbb{C}^{q \times q}[\xi]$, $i = 0, 1, \dots, n-1$ as used in (2). In particular, let $\varphi_i(\xi)$ be decomposed into individual vector-polynomials, i.e.,

$$\varphi_i(\xi) = [\underline{\varphi}_{(i+0)}(\xi), \underline{\varphi}_{(i+1)}(\xi), \dots, \underline{\varphi}_{(i+q)}(\xi)].$$

Then, element (e_1, e_2) of $\langle\langle \varphi_i(\xi), \varphi_j(\xi) \rangle\rangle$ is given by

$$\langle \underline{\varphi}_\kappa(\xi), \underline{\varphi}_\ell(\xi) \rangle := \sum_{k=1}^m \underline{\varphi}_\ell(\xi_k)^H w_{1k}^H w_{1k} \underline{\varphi}_\kappa(\xi_k), \quad (22)$$

where $\kappa = i + e_2$ and $\ell = j + e_1$. Indeed, (19) is consistent with the theory in [7, Sect. 1.1–1.2] and [10], [45].

Note that in the general case in Lemma 13-(c), the vector-polynomial bases $\varphi(\xi)$ and $\psi(\xi)$ may be distinct. In the next section, it is shown that by choosing polynomial bases that are bi-orthonormal with respect to (21), a solution of the polynomial equality (1) similar to (20) is obtained, which facilitates an accurate numerical computation.

B. Achieving optimal numerical conditioning through the use of bi-orthonormal polynomial bases

The aim in this paper is to solve the polynomial equality (1) through a polynomial approach that inherently has optimal numerical conditioning. As motivated in Sect. III-C, the selection

of the basis in which the problem is formulated is a crucial step that determines the solution accuracy. For the general problem (1), there is freedom to select two polynomial bases $\varphi_j(\xi)$ and $\psi_j(\xi)$, which constitute the polynomials $f(\xi, \theta)$ and $g(\xi, \theta)$ in (2)–(3), respectively. The following definition is at the basis of subsequent developments.

Definition 15. Let $\xi_k \in \mathbb{C}$ and $w_{1k}, w_{2k} \in \mathbb{C}^{1 \times q}$, $k = 1, \dots, m$, be given. In addition, let $\varphi_i(\xi), \psi_j(\xi) \in \mathbb{C}^{q \times q}[\xi]$, $i, j = 0, 1, \dots, n$. Then, $\varphi_i(\xi), \psi_j(\xi)$ are called *bi-orthonormal block-polynomials (BBPs)* with respect to (21) if:

$$\llbracket \varphi_i(\xi), \psi_j(\xi) \rrbracket := \sum_{k=1}^m \psi_j(\xi_k)^H w_{2k}^H w_{1k} \varphi_i(\xi_k) = \delta_{ij} I_q. \quad (23)$$

A key new result of this paper is the selection of two *distinct, bi-orthonormal* polynomial bases. By formulating the polynomial equation (1) in bi-orthonormal polynomial bases, the following remarkable main result is obtained.

Theorem 16. Consider (1), where $f(\xi, \theta), g(\xi, \theta)$ defined in (2)–(3) are formulated in polynomial bases $\varphi_i(\xi), \psi_j(\xi) \in \mathbb{C}^{q \times q}[\xi]$, $i, j = 0, 1, \dots, n$ that satisfy (23). Then, the solution $f(\xi, \theta)$ to (1) is given by:

$$f(\xi, \theta) = f_n(\xi) = \varphi_n(\xi) \theta_n, \quad (24)$$

where f_n is defined in (9).

Proof: Consider the reformulation of (1) as the oblique projection (13), where the matrix $\Psi^H W_2^H W_1 \Phi_n \in \mathbb{C}^{nq \times nq}$ is of importance here. Since the $q \times q$ -block-element $(j, 1)$ of this matrix is equal to $\llbracket \varphi_n(\xi), \psi_j(\xi) \rrbracket$, it follows by virtue of orthogonality of $\varphi_n(\xi)$ and $\psi_j(\xi)$, $j = 0, 1, \dots, n-1$, that

$$\Psi^H W_2^H W_1 \Phi_n = 0. \quad (25)$$

As a consequence of (25), the solution for the parameter vector $\theta = [\theta_0^T \ \theta_1^T \ \dots \ \theta_{n-1}^T]^T$, in (13) equals $\theta = 0$. Therefore, (2) reduces to (24), where θ_n has been selected according to (7) to impose a degree constraint on $f(\xi, \theta)$. ■

Theorem 16 implies that, given bi-orthonormal polynomial bases with respect to the *data-dependent* bi-linear form (21), the solution to the polynomial equation (1) is immediate. In terms of the associated linear system of equations (13), the following result is obtained.

Theorem 17. Consider (13). Let $\varphi_i(\xi), \psi_j(\xi) \in \mathbb{C}^{q \times q}[\xi]$, $i, j = 0, 1, \dots, n$ be bi-orthonormal with respect to (21), cf. Def. 15. Then,

$$\Psi^H W_2^H W_1 \Phi = I, \quad (26)$$

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

Proof: Follows directly from bi-orthonormality of $\varphi_i(\xi), \psi_j(\xi) \in \mathbb{C}^{q \times q}[\xi]$, $i, j = 0, 1, \dots, n$, which can be rewritten in matrix form as (26). ■

In conclusion, selection of appropriate, problem specific polynomial bases yields an optimally conditioned linear algebra problem. In contrast, the use of different polynomial bases generally leads to $\kappa(\Psi^H W_2^H W_1 \Phi) \gg 1$, see Sect. V-B and [6] for special case of orthonormal polynomials.

Through the use of BBPs, Thm. 16. reveals that (13) need not be solved explicitly anymore. Thus, it remains to construct the BBPs with respect to (21). Before presenting the construction of these BBPs, the need for considering *two distinct* polynomial bases instead of using a single one is proved.

C. Connecting bi-orthonormality and asymmetry of the polynomial approximation problem

In this section, it is shown that there are fundamental relations between the asymmetry of the polynomial approximation problem (1) and bi-orthonormal polynomials. To facilitate the presentation of the main ideas, attention is restricted to *real-valued* polynomial approximation problems in this section. Extensions for complex values follow along the same lines.

Assumption 18. In this section, $\xi_k \in \mathbb{R}$, $w_{1k}, w_{2k} \in \mathbb{R}^{1 \times q}$, $k = 1, \dots, m$. Furthermore, $\varphi_i(\xi), \psi_j(\xi) \in \mathbb{R}^{q \times q}[\xi]$, $i, j = 0, 1, \dots, n-1$.

To present the main results, it is convenient to relax the notion of bi-orthonormality in Def. 15 to *bi-orthogonality*, which is defined in matrix form as

$$\Psi^T W_2 W_1 \Phi = D, \quad (27)$$

with $D \in \mathbb{R}^{nq \times nq}$ a diagonal matrix. The main difference with Def. 15 is thus a normalization step. Next, the form (27) is used to show that it cannot be achieved for general weights $w_{1k} \neq w_{2k}$, $k = 1, \dots, m$ with $\psi_j(\xi) = \varphi_j(\xi)$, $j = 0, 1, \dots, n-1$. The following definition is used to formulate the main result.

Definition 19. Let nonzero $\xi_k \in \mathbb{R}$ and $w_{1k}, w_{2k} \in \mathbb{R}^{1 \times q}$, $k = 1, \dots, m$, be given. For $i, j = 0, 1, \dots, n-1$, with $n < m$, define

$$\mathcal{S}_{ij} = \sum_{k=1}^m \xi_k^{(i+j)} \cdot (w_{2k}^T w_{1k} - w_{1k}^T w_{2k}) \in \mathbb{R}^{q \times q}.$$

Remark 20. If $w_{2k}^T w_{1k}$ is symmetric for all $k = 1, \dots, m$, i.e., $w_{2k}^T w_{1k} = w_{1k}^T w_{2k}$, then $\mathcal{S}_{ij} = 0 \ \forall i, j = 0, 1, \dots, n-1$. A particular example hereof is obtained when $w_{1k}, w_{2k} \in \mathbb{R}$ are scalar.

The following theorem is the main result of this section and connects the asymmetry of the weights $w_{2k}^T w_{1k}$ to bi-orthonormal polynomials.

Theorem 21. Let $\xi_k \in \mathbb{R}$ and $w_{1k}, w_{2k} \in \mathbb{R}^{1 \times q}$, $k = 1, \dots, m$, be given and let $W_1, W_2 \in \mathbb{R}^{m \times m q}$ be defined in (16). Furthermore, let $D \in \mathbb{R}^{nq \times nq}$ be a diagonal matrix. Then, there exists a polynomial basis $\varphi_j(\xi) \in \mathbb{R}^{q \times q}[\xi]$, $j = 0, 1, \dots, n-1$ with corresponding matrix Φ defined in (14) such that

$$\Phi^T W_2^T W_1 \Phi = D \quad (28)$$

if and only if $\mathcal{S}_{ij} = 0 \ \forall i, j = 0, 1, \dots, n-1$.

Theorem 21 shows that i) for *asymmetric* weights $w_{2k}^T w_{1k}$, $k = 1, \dots, m$, two *distinct* polynomial bases are required in order to achieve bi-orthogonality with respect to the general

bi-linear form (21), whereas ii) for *symmetric positive definite* weights $w_{1k}^T w_{1k}$, as encountered in the inner product (22), it is possible to achieve orthogonality with a *single* polynomial basis, since in that case $\mathcal{S}_{ij} = 0 \forall i, j = 0, 1, \dots, n-1$, see Remark 20. In particular, the special case of symmetric positive definite weights has been considered in [30], [5], [11], [21], where orthonormal polynomials with respect to a data-dependent inner product have been introduced to solve (11).

Finally, attention is turned to the specific class of indefinite inner products, see Fig. 1. From Lemma 13-(b) it follows that, while the bi-linear form (21) is symmetric in this case, i.e., $w_{2k}^T w_{1k} = w_{1k}^T w_{2k}$, the matrices $w_{2k}^H w_{1k}$, $k = 1, \dots, m$ may be indefinite. Nevertheless, for this special sub-class of the general bi-linear form it is possible to achieve the results in Thm. 16 and Thm. 17 using a *single* polynomial basis. Therefore, the definition of bi-orthonormality for block-polynomials, see Def. 15, needs to be extended as follows.

Definition 22. Let $\xi_k \in \mathbb{R}$ and $w_{1k}, w_{2k} \in \mathbb{R}^{1 \times q}$, $k = 1, \dots, m$, be given. Moreover, let $w_{2k}^T w_{1k} = w_{1k}^T w_{2k}$. Finally, let $[\cdot, \cdot]$ be defined in (23). Then, $\varphi_i(\xi) \in \mathbb{R}^{q \times q}[\xi]$, $i = 0, 1, \dots, n$ are called *orthonormal with respect to the indefinite inner product* (21) if

$$[\varphi_i(\xi), \varphi_j(\xi)] = \delta_{ij} D_{ij}, \quad (29)$$

where $D_{ii} = \text{diag}(\pm 1, \pm 1, \dots, \pm 1) \in \mathbb{R}^{q \times q}$.

In this definition of orthonormality for indefinite inner products, see also [14, Sect. 2.2], the righthand side of (29) accounts for the fact that the matrices $w_{2k}^H w_{1k}$, $k = 1, \dots, m$ may be indefinite. Indeed, by exploiting a polynomial basis that obeys the orthonormality condition in Def. 22, both Thm. 16 and Thm. 17 hold using a *single* basis, irrespective of the *indefinite* character of (21).

In conclusion, the *asymmetry* of weights in (1) necessitates the construction of two distinct polynomial bases. In the remainder of this paper, the construction of bi-orthonormal polynomial bases is considered in detail. This covers the case of indefinite and standard inner products as a special case, see Fig. 1. Thus, the developed theory covers these cases. Note that by exploiting symmetry, the results for the special cases may be simplified.

V. A THEORY FOR BI-ORTHONORMAL POLYNOMIALS

In this section a theory is developed for the construction of bi-orthonormal polynomials. Starting from a linear algebra perspective, in Sect. V-A, the oblique projection (13) is studied in more detail, leading to a connection with two Krylov subspaces in Sect. V-B. Next, in Sect. V-C, it is shown that bi-orthonormal bases for these two Krylov subspaces are directly connected with the bi-orthonormal polynomials that need to be constructed. This finally leads to a derivation of three-term-recurrence relations for bi-orthonormal polynomials in Sect. V-D, in which the recurrence coefficients are connected to given problem data.

A. Properties of the oblique projection

An oblique projection, see, e.g., [2, Sect. 3], [33, Sect. 5.2], is characterized by two subspaces that define its range and

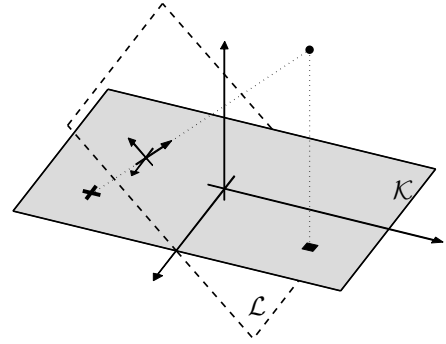


Fig. 2. Two projections of (●) onto subspace \mathcal{K} : orthogonal projection (■) and oblique projection (×) with residual orthogonal to subspace \mathcal{L} .

null-space. As is illustrated in Fig. 2, a given point in space is projected *onto* a subspace \mathcal{K} , *along* a line orthogonal to a subspace \mathcal{L} . In other words, the residual is orthogonal to \mathcal{L} .

By rewriting the oblique projection (13) in Sect. III-A as

$$\Psi^H W_2^H (W_1 \Phi \theta + W_1 \Phi_n \theta_n) = 0,$$

it is observed that, in view of (18),

- 1) the vector $-W_1 \Phi_n \theta_n$ is projected onto the subspace $\mathcal{K} := \text{span}(W_1 \Phi)$, on which θ operates, and
- 2) the residual $(W_1 \Phi \theta + W_1 \Phi_n \theta_n)$ is orthogonal to the subspace $\mathcal{L} := \text{span}(W_2 \Psi)$.

Remark 23. The oblique projector is given by the mapping $P_{\text{obl}} : -W_1 \Phi_n \theta_n \mapsto W_1 \Phi \theta$, where, using (13),

$$P_{\text{obl}} = W_1 \Phi (\Psi^H W_2^H W_1 \Phi)^{-1} \Psi^H W_2^H. \quad (30)$$

Clearly, $P_{\text{obl}}^2 = P_{\text{obl}}$, and hence indeed is a projector.

The results from Sect. IV are now reinterpreted. Importantly, the oblique projector (30) is *asymmetric*, since (13) is characterized by two distinct subspaces. To achieve optimal numerical conditioning of (13), it is needed to account for this asymmetry explicitly, which will be done by developing *two distinct* bases for these subspaces.

In the special situation where \mathcal{K} and \mathcal{L} coincide, an orthogonal projection is obtained.

Lemma 24. A projector is orthogonal if and only if it is Hermitian.

Proof: A proof is given in [33, Sect. 1.12.3]. ■

In particular, \mathcal{K} and \mathcal{L} coincide if $W_2 = W_1$ and $\Psi = \Phi$, cf. Remark 9. Indeed, the resulting *orthogonal projector*

$$P_{\text{orth}} = W_1 \Phi (\Phi^H W_1^H W_1 \Phi)^{-1} \Phi^H W_1^H$$

is Hermitian. In this special situation, (13) reduces to the orthogonal projection (17), for which optimal numerical conditioning is attained with a single basis, cf. Sect. III-C.

B. Defining the oblique projection through Krylov subspaces

In this section, it is shown that due to an imposed degree structure, \mathcal{K} and \mathcal{L} are Krylov subspaces. The following simplifying assumption is made. However, the entire theory can be extended to the general situation along similar lines.

Assumption 25. To facilitate the presentation, $q = 1$ and $\xi_k, w_{1k}, w_{2k} \in \mathbb{R}$, $k = 1, \dots, m$ in the remainder of this paper.

By virtue of the degree structure in Ass. 4, the polynomials $\varphi_j(\xi), \psi_j(\xi), j = 0, 1, \dots, n-1$, in (5)–(6) can be expressed as a linear combination of $\phi_{\text{mon},j}(\xi)$ in (4), viz.

$$\begin{aligned}\varphi_j(\xi) &= \sum_{k=0}^j s_{jk} \phi_{\text{mon},k}(\xi), \quad s_{jk} \in \mathbb{R}, \quad k = 0, \dots, j, \\ \psi_j(\xi) &= \sum_{k=0}^j t_{jk} \phi_{\text{mon},k}(\xi), \quad t_{jk} \in \mathbb{R}, \quad k = 0, \dots, j,\end{aligned}$$

where s_{jj}, t_{jj} are non-zero by assumption. As a result, Φ and Ψ in (14)–(15) can be written as

$$\Phi = V S, \quad (31)$$

$$\Psi = V T, \quad (32)$$

$$V = \begin{bmatrix} 1 & \xi_1 & \dots & \xi_1^{n-1} \\ 1 & \xi_2 & \dots & \xi_2^{n-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \xi_m & \dots & \xi_m^{n-1} \end{bmatrix} S = \begin{bmatrix} s_{0,0} & \dots & s_{n-1,0} \\ & \ddots & \vdots \\ & & s_{n-1,n-1} \end{bmatrix} T = \begin{bmatrix} t_{0,0} & \dots & t_{n-1,0} \\ & \ddots & \vdots \\ & & t_{n-1,n-1} \end{bmatrix}. \quad (33)$$

Here, $V \in \mathbb{R}^{m \times n}$ is a Vandermonde matrix and $S, T \in \mathbb{R}^{n \times n}$ are invertible upper triangular matrices. The particular structure of (31)–(32) is used to formulate the main result of this section, which shows that \mathcal{K} and \mathcal{L} are Krylov subspaces.

Definition 26. [15, Sect. 7.4.5] A Krylov subspace $\mathcal{K}_n(A, b)$ generated by $A \in \mathbb{R}^{m \times m}$ and $b \in \mathbb{R}^{m \times 1}$ is defined as

$$\mathcal{K}_n(A, b) = \text{span}\{b, Ab, A^2b, \dots, A^{n-1}b\}.$$

Remark 27. The Vandermonde matrix V in (33) is an elementary Krylov matrix, which reflects the degree structure of the monomial basis in (4).

Lemma 28. Let Φ, Ψ be defined in (14)–(15) and W_1, W_2 in (16). Then,

$$\mathcal{K} := \text{span}(W_1 \Phi) \quad (34)$$

$$\mathcal{L} := \text{span}(W_2 \Psi) \quad (35)$$

are Krylov subspaces.

Proof: By virtue of (31)–(32), with S and T invertible, $\text{span}(W_1 \Phi) = \text{span}(W_1 V)$ and $\text{span}(W_2 \Psi) = \text{span}(W_2 V)$. Now, observe that it is possible to write

$$W_1 V = K := [W_1 \quad XW_1 \quad \dots \quad X^{n-1}W_1] \in \mathbb{R}^{m \times n}, \quad (36)$$

$$W_2 V = L := [W_2 \quad XW_2 \quad \dots \quad X^{n-1}W_2] \in \mathbb{R}^{m \times n}, \quad (37)$$

with node matrix X and weight vectors $\underline{W}_1, \underline{W}_2$ given by

$$X = \text{diag}(\xi_1, \xi_2, \dots, \xi_m) \in \mathbb{R}^{m \times m} \quad (38)$$

$$\underline{W}_1 = [w_{11} \quad w_{12} \quad \dots \quad w_{1m}]^T \in \mathbb{R}^{m \times 1}, \quad (39)$$

$$\underline{W}_2 = [w_{21} \quad w_{22} \quad \dots \quad w_{2m}]^T \in \mathbb{R}^{m \times 1}.$$

From Def. 26 it follows that K and L form a Krylov basis, which completes the proof. ■

Lemma 28 shows that for any choice of basis polynomials $\varphi_j(\xi), \psi_j(\xi), j = 0, 1, \dots, n-1$ that satisfy a degree structure, the subspaces \mathcal{K} and \mathcal{L} defining the oblique projection (13) are Krylov subspaces. Projection methods on Krylov subspaces have been studied in, e.g., [23], [25], [32].

If the monomial basis $\phi_{\text{mon},j}(\xi)$ in (4) is used for $\varphi_j(\xi)$ and $\psi_j(\xi)$, i.e., K and L in (36)–(37) are used as a vector basis for \mathcal{K} and \mathcal{L} , then (13) takes the form:

$$(L^T K) \theta = (V^T W_2^T W_1 V) \theta = V^T W_2^T W_1 \Phi_n \theta_n. \quad (40)$$

Typically, (40) is severely ill-conditioned, i.e., $\kappa(L^T K) \gg 1$. On the contrary, the use of bi-orthonormal polynomial bases for $\varphi_j(\xi)$ and $\psi_j(\xi)$ leads to optimal conditioning of the oblique projection (13), see Sect. IV. The next section shows that optimal conditioning is in fact achieved by using bi-orthonormal vector-bases for \mathcal{K}, \mathcal{L} .

C. Bi-orthonormal vector-bases for Krylov subspaces

In this section, it is shown that formulating the oblique projection (13) using bi-orthonormal polynomials yields bi-orthonormal vector-bases for the Krylov subspaces \mathcal{K}, \mathcal{L} . Furthermore, these bases are shown to be related to an important matrix tri-diagonalization problem.

The following theorem connects bi-orthonormal polynomials with bi-orthonormal Krylov bases.

Theorem 29. Let $\varphi_j(\xi), \psi_j(\xi) \in \mathbb{R}[\xi], j = 0, 1, \dots, n-1$, be bi-orthonormal polynomials, see Def. 15. Let $S, T \in \mathbb{R}^{n \times n}$ be the coefficient matrices of these polynomials, such that (31)–(32) hold. Now, using (36)–(37), define

$$\tilde{K} := K S = W_1 V S, \quad (41)$$

$$\tilde{L} := L T = W_2 V T,$$

Then, bi-orthonormality of $\varphi_j(\xi), \psi_j(\xi), j = 0, 1, \dots, n-1$, implies that

$$\tilde{L}^T \tilde{K} = I.$$

Proof: By virtue of Thm. 17 for bi-orthonormal polynomials, S and T are such that:

$$\tilde{L}^T \tilde{K} = T^T V^T W_2^T W_1 V S = \Psi^T W_2^T W_1 \Phi = I. \quad \blacksquare$$

Remark 30. The first columns of \tilde{K} and \tilde{L} are obtained by normalizing the weight vectors \underline{W}_1 and \underline{W}_2 :

$$\tilde{k}_1 = \underline{W}_1 / \sqrt{|\underline{W}_2^T \underline{W}_1|}, \quad (42)$$

$$\tilde{l}_1 = \text{sign}(\underline{W}_2^T \underline{W}_1) \cdot \underline{W}_2 / \sqrt{|\underline{W}_2^T \underline{W}_1|}. \quad (43)$$

Since \tilde{K}, \tilde{L} reflect the degree structure of $\varphi_j(\xi), \psi_j(\xi), j = 0, 1, \dots, n-1$, these Krylov bases have a remarkable connection with a matrix tri-diagonalization problem. The following lemmas are used to formulate the main result.

Lemma 31. Let X and $\underline{W}_1, \underline{W}_2$ be defined in (38)–(39). Let \tilde{K}, \tilde{L} denote bi-orthonormal vector-bases for \mathcal{K}, \mathcal{L} in (34)–(35), respectively, with \tilde{k}_1, \tilde{l}_1 defined in (42)–(43). Then,

$$\tilde{L}^T X \tilde{K} = H_1,$$

where H_1 denotes an upper Hessenberg matrix.

In analogy to Lemma 31, the following result holds.

Lemma 32. *Let X and $\underline{W}_1, \underline{W}_2$ be defined in (38)–(39). Let \tilde{K}, \tilde{L} denote bi-orthonormal vector-bases for \mathcal{K}, \mathcal{L} in (34)–(35), respectively, with \tilde{k}_1, \tilde{l}_1 defined in (42)–(43). Then,*

$$\tilde{K}^T X \tilde{L} = H_2,$$

where H_2 denotes an upper Hessenberg matrix.

Together, Lemma 31 and Lemma 32 provide the basis to relate bi-orthonormal Krylov bases vectors with a matrix tri-diagonalization problem. For the following result, assume that $n = m$, with m the number of nodes in (1), such that the Krylov subspaces \mathcal{K} and \mathcal{L} in (34)–(35) span $\mathbb{R}^{m \times m}$.

Theorem 33. *Let X and $\underline{W}_1, \underline{W}_2$ be defined in (38)–(39). Let \tilde{K}, \tilde{L} denote bi-orthonormal vector-bases that span \mathcal{K}, \mathcal{L} in (34)–(35), respectively, with \tilde{k}_1, \tilde{l}_1 defined in (42)–(43). Then, the pair $\tilde{K}, \tilde{L} = \tilde{K}^{-T}$ induces a similarity transformation, which transforms an initial node-weight matrix into tri-diagonal form as follows:*

$$\begin{bmatrix} 1 & \\ & \tilde{L}^T \end{bmatrix} \left[\begin{array}{c|c} 0 & \underline{W}_2^T \\ \underline{W}_1 & X \end{array} \right] \begin{bmatrix} 1 & \\ & \tilde{K} \end{bmatrix} = \left[\begin{array}{c|c} 0 & \beta_0 \ 0_{1,m-1} \\ \gamma_0 & \mathcal{T} \\ 0_{m-1,1} & \end{array} \right], \quad (44)$$

where

$$H_1 = H_2^T = \begin{bmatrix} \alpha_1 & \beta_1 & & & & \\ \gamma_1 & \alpha_2 & \beta_2 & & & \\ & \gamma_2 & \ddots & \ddots & & \\ & & \ddots & \ddots & \beta_{m-1} & \\ & & & \gamma_{m-1} & \alpha_m & \end{bmatrix} := \mathcal{T}. \quad (45)$$

Remark 34. *Note that (44) can only be attained for $\xi_k, w_{1k}, w_{2k} \in \mathbb{R}$, see Ass. 18. For general $\xi_k, w_{1k}, w_{2k} \in \mathbb{C}$, two distinct Hessenberg matrices H_1 and H_2 are obtained.*

Theorem 33 is connected with Lanczos' algorithm [25], to convert a non-symmetric matrix into a tri-diagonal matrix under similarity. In turn, Lanczos' algorithm can be considered as special variant of the conjugate-gradient method [23]. Matrix tri-diagonalization is also studied in, e.g., [43], [33].

Starting from (44), three-term-recurrence relations for bi-orthonormal polynomials can be derived, as explained next.

D. Three-term-recurrence relations

In this section, three-term-recurrence relations for bi-orthonormal polynomials are derived. First, it is shown that (44) enables the derivation of three-term-recurrence relations for the columns of the Krylov bases \tilde{K} and \tilde{L} , see also [32].

Lemma 35. *Consider the similarity transformation (44) in Thm. 33. The columns of the matrices \tilde{K} and \tilde{L} satisfy the following three-term-recurrence relations:*

$$\tilde{k}_{j+1} = \frac{1}{\gamma_j} ((X - \alpha_j) \tilde{k}_j - \beta_{j-1} \tilde{k}_{j-1}), \quad (46)$$

$$\tilde{l}_{j+1} = \frac{1}{\beta_j} ((X - \alpha_j) \tilde{l}_j - \gamma_{j-1} \tilde{l}_{j-1}). \quad (47)$$

The three-term-recurrence relations (46)–(47) are initialized with \tilde{k}_1 and \tilde{l}_1 in (42)–(43) and $\tilde{k}_0 := 0, \tilde{l}_0 := 0$.

An intrinsic relation exists between bi-orthonormal Krylov bases \tilde{K} and \tilde{L} and bi-orthonormal polynomials $\varphi_j(\xi), \psi_j(\xi), j = 0, \dots, n-1$. This is confirmed in the following theorem, where Lemma 35 is used to derive three-term-recursion relations for bi-orthonormal polynomials.

Theorem 36. *Consider the similarity transformation (44) in Thm. 33. Bi-orthonormal polynomials $\varphi_j(\xi), \psi_j(\xi), j = 0, \dots, n-1$ with respect to the bi-linear form (13) for the considered nodes and weights satisfy the following three-term-recurrence relations:*

$$\varphi_j(\xi) = \frac{1}{\gamma_j} ((\xi - \alpha_j) \varphi_{j-1}(\xi) - \beta_{j-1} \varphi_{j-2}(\xi)), \quad (48)$$

$$\psi_j(\xi) = \frac{1}{\beta_j} ((\xi - \alpha_j) \psi_{j-1}(\xi) - \gamma_{j-1} \psi_{j-2}(\xi)). \quad (49)$$

Three-term-recurrence relations for bi-orthonormal polynomials are also studied in, e.g., [17], [12].

Given the recursion coefficients that form the tri-diagonal matrix \mathcal{T} in (45), (48)–(49) enable the efficient construction of $\varphi_j(\xi), \psi_j(\xi), j = 0, 1, \dots, n-1$. Hence, the essence of constructing bi-orthonormal polynomial bases is a numerically accurate and efficient algorithm for performing the matrix tri-diagonalization in (44). Such an algorithm is presented next.

VI. ALGORITHM FOR RECURRENCE COEFFICIENTS

In this section, an algorithm is developed to solve the matrix tri-diagonalization problem (44). First, in Sect. VI-A, a special tri-diagonal form is considered. Then, in Sect. VI-B, an algorithm that extends the 'chasing down the diagonal' approach in [30] and [37] is presented.

A. Special tri-diagonal matrix for an indefinite inner product

Matrix tri-diagonalization (44) is obtained by virtue of Ass. 18, which implies that

$$w_{2k}^T w_{1k} = w_{1k}^T w_{2k} \in \mathbb{R}, \quad k = 1, \dots, m.$$

In that case, (21) is symmetric and defines an indefinite inner product, cf. Lemma 13-(b). As shown in Sect. IV-C, the main results in Thm. 16 and Thm. 17 can now be attained using a *single* polynomial basis, which is obtained by employing the general theory in Sect. V.

Importantly, (44) is non-unique, since bi-orthogonal pairs $\tilde{k}_j, \tilde{l}_j, j = 0, 1, \dots, m$ can be scaled arbitrarily to obtain $\tilde{l}_j^T \tilde{k}_j = 1$. This property is exploited to construct a special tri-diagonal matrix \mathcal{T}_s that has i) positive sub-diagonal elements, and ii) super-diagonal elements that are equal in magnitude to the sub-diagonal elements, but may have opposite sign, see also [32, p. 487]. Hereby, an interesting result is obtained.

Lemma 37. *Consider (44). Let $\gamma_j > 0, j = 0, 1, \dots, m-1$. In addition, let $|\beta_j| = \gamma_j$, i.e., $\beta_j = \pm \gamma_j, j = 0, 1, \dots, m-1$. Thus, the tri-diagonal matrix takes the special form*

$$\mathcal{T}_s = \begin{bmatrix} \alpha_1 & \pm\gamma_1 & & & & \\ \gamma_1 & \alpha_2 & \pm\gamma_2 & & & \\ & \gamma_2 & \alpha_3 & \ddots & & \\ & & \ddots & \ddots & \pm\gamma_{k-1} & \\ & & & & \gamma_{k-1} & \alpha_k \end{bmatrix}. \quad (50)$$

Now, let bi-orthonormal polynomials $\varphi_i(\xi), \psi_j(\xi)$, $i, j = 0, 1, \dots, n-1$ be constructed using (48)–(49), with initialization (70)–(71). Then,

$$\psi_j(\xi) = \pm \varphi_j(\xi) \quad \forall j = 0, 1, \dots, n-1. \quad (51)$$

Result (51) has an important implication for the bi-orthonormal bases that are developed using (50).

Theorem 38. Consider (44), where the tri-diagonal matrix takes the form \mathcal{T}_s in (50). Let bi-orthonormal polynomial bases φ_i, ψ_j , $i, j = 0, 1, \dots, n-1$ be generated by (48)–(49), with recurrence coefficients taken from \mathcal{T}_s . Then, the individual polynomial basis $\varphi_i(\xi)$, $i = 0, 1, \dots, n-1$, as well as the polynomial basis $\psi_j(\xi)$, $j = 0, 1, \dots, n-1$, is orthonormal with respect to the indefinite inner product (21).

Theorem 38 confirms that a polynomial basis that is orthonormal with respect to an indefinite inner product is obtained *immediately* by pursuing the general theory for bi-orthonormal polynomial bases. The next section provides an algorithm to construct the form (50).

B. Chasing down the diagonal

In this section, a numerically reliable algorithm is presented that develops the decomposition (44) for the tri-diagonal form (50). This algorithm follows the rationale of ‘chasing down the diagonal’, pursued in [31], [30], and [37]. In particular, new node-weights triples are added to the problem one by one, after which the intermediate result is converted into a tri-diagonal matrix of appropriate size. As a result, i) the underlying structure of the problem can be exploited, and ii) numerical round-off errors are minimal. The main steps of the algorithm are as follows.

Algorithm 39 (Chasing down the diagonal).

Initialization: Using (ξ_1, w_{11}, w_{12}) , define the initial matrix

$$\begin{bmatrix} \beta_1 \\ \gamma_1 & \alpha_1 \end{bmatrix} = \begin{bmatrix} \text{sign}(w_{11}w_{21})\sqrt{|w_{11}w_{21}|} & \\ \sqrt{|w_{11}w_{21}|} & \xi_1 \end{bmatrix}.$$

Addition of new node-weights triple: Starting with $k = 1$, consider the k^{th} tri-diagonal matrix, which is appended with the $(k+1)^{\text{th}}$ node-weights triple (ξ_k, w_{1k}, w_{2k}) :

$$S_0 = \begin{bmatrix} & & w_{2k} & \pm\gamma_0 & & & \\ & & \xi_k & & & & \\ w_{1k} & & & \alpha_1 \pm \gamma_1 & & & \\ \pm\gamma_0 & & & \gamma_1 & \alpha_2 \pm \gamma_2 & & \\ & & & \gamma_2 & \alpha_3 & \ddots & \\ & & & & \ddots & \ddots & \pm\gamma_{k-1} \\ & & & & & \gamma_{k-1} & \alpha_k \end{bmatrix}.$$

Two steps are taken to zero the indicated elements that violate the structure of a tri-diagonal matrix under similarity.

• Step 1:

Re-scaling of the new weights, to introduce symmetry up to minus signs. Let $\varsigma_1 = \text{sign}(w_{1k})$, and define

$$P_0 = \begin{bmatrix} 1 & & & \\ & \varsigma_1 \cdot \sqrt{\left| \frac{w_{2k}}{w_{1k}} \right|} & & \\ & & I_k & \\ & & & 1 \end{bmatrix}, \quad Q_0 = \begin{bmatrix} 1 & & & \\ & \varsigma_1 \cdot \sqrt{\left| \frac{w_{1k}}{w_{2k}} \right|} & & \\ & & I_k & \\ & & & 1 \end{bmatrix}.$$

Then,

$$S_1 = P_0^T S_0 Q_0 =$$

$$\begin{bmatrix} & & \pm\sqrt{|w_{1k}w_{2k}|} & \pm\gamma_0 & & & \\ \sqrt{|w_{1k}w_{2k}|} & & \xi_k & & & & \\ \pm\gamma_0 & & & \alpha_1 \pm \gamma_1 & & & \\ & & & \gamma_1 & \alpha_2 \pm \gamma_2 & & \\ & & & & \gamma_2 & \alpha_3 & \ddots \\ & & & & & \ddots & \ddots & \pm\gamma_{k-1} \\ & & & & & & \gamma_{k-1} & \alpha_k \end{bmatrix}.$$

• Step 2:

Chasing the bulge elements down the diagonal, where the indicated window ①, ②, ... is shifted down along the main diagonal. Let window j be updated as follows:

$$P_j^T \begin{bmatrix} \alpha'_{j-1} & \mu & \rho \\ \nu & \lambda & \sigma \\ \pi & \tau & \alpha_j & \beta_j \\ & & \gamma_j & \alpha_{j+1} \end{bmatrix} Q_j = \begin{bmatrix} \alpha'_{j-1} & \beta'_{j-1} & & & \\ \gamma'_{j-1} & \alpha'_j & \mu' & \rho' \\ & \nu' & \lambda' & \sigma' \\ & & \pi' & \tau' & \alpha_{j+1} \end{bmatrix},$$

where the similarity transformation matrices $P_j, Q_j \in \mathbb{R}^{4 \times 4}$, for which holds that $P_j^T Q_j = I$, are given by

$$P_j = \begin{bmatrix} 1 & & & \\ \varsigma \cdot \frac{\mu}{\gamma'_{j-1}} & \varsigma \cdot \frac{\pi}{\gamma'_{j-1}} & & \\ \varsigma \cdot \frac{\rho}{\gamma'_{j-1}} & \varsigma \cdot \frac{\nu}{\gamma'_{j-1}} & & \\ & & & 1 \end{bmatrix}, \quad Q_j = \begin{bmatrix} 1 & & & \\ \frac{\nu}{\gamma'_{j-1}} & \frac{\rho}{\gamma'_{j-1}} & & \\ \frac{\pi}{\gamma'_{j-1}} & \frac{-\mu}{\gamma'_{j-1}} & & \\ & & & 1 \end{bmatrix},$$

with $\gamma'_{j-1} = \sqrt{|\pi\rho + \nu\mu|}$ and $\varsigma = \text{sign}(\pi\rho + \nu\mu)$. It is readily verified that as a result, $0 < \gamma'_{j-1} = \pm\beta'_{j-1}$. ■

Generalizations of Alg. 39 for the situation where $\xi_k \in \mathbb{C}$, $w_{1k}, w_{2k} \in \mathbb{C}^{1 \times q}$, $k = 1, \dots, m$, with $q > 1$, follow the same philosophy as presented above.

Remark 40. Note that in the situation where $w_{2k} = w_{1k} \forall k = 1, \dots, m$, i.e., (21) defines a conventional inner product, P_j and Q_j coincide and form the Givens reflector

$$P_j = Q_j = \begin{bmatrix} 1 & & & \\ \frac{\mu}{\sqrt{\pi^2 + \mu^2}} & \frac{\pi}{\sqrt{\pi^2 + \mu^2}} & & \\ \frac{\pi}{\sqrt{\pi^2 + \mu^2}} & \frac{-\mu}{\sqrt{\pi^2 + \mu^2}} & & \\ & & & 1 \end{bmatrix},$$

In that case, Alg. 39 reduces to the algorithm in [31] and [16] with established good numerical properties, which transforms a symmetric node-weights matrix into Jacobi form under unitary similarity. In the general case, P_j and Q_j are not unitary, although $\det(P_j) = \det(Q_j) = 1$, except for the scaling transformation P_0, Q_0 . A full analysis of Alg. 39 is beyond the scope of this paper.

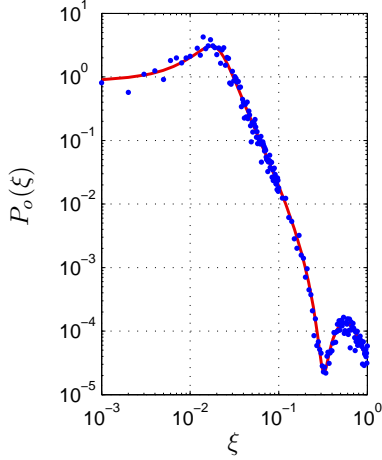


Fig. 3. Noisy measurements $P_o(\xi_k), k = 1, \dots, 190$, of the true system.

VII. NUMERICAL EXAMPLE

A. Problem setup

In this section, the main result of this paper is illustrated on a simulation example. A 6th order true system $P_o(\xi) = \frac{n_o(\xi)}{d_o(\xi)} = 10^4 \cdot \frac{59.37 \xi^4 - 151.16 \xi^3 + 134.09 \xi^2 - 47.15 \xi + 5.72}{\xi^6 + 1.11 \cdot 10^2 \xi^4 + 1.67 \cdot 10^8 \xi^2 - 5.91 \cdot 10^6 \xi + 6.85 \cdot 10^4}$ is considered, with $\xi \in \mathbb{R}$. It is assumed that the true numerator $n_o(\xi)$ is known. Hence, a model $\hat{P}(\xi, \theta)$ is parametrized as

$$\hat{P}(\xi, \theta) = \frac{n_o(\xi)}{d(\xi, \theta)}, \quad d(\xi, \theta) = \sum_{j=0}^6 \varphi_j(\xi) \theta_j,$$

where $\varphi_j(\xi) \in \mathbb{R}[\xi]$ is a scalar, degree j , real polynomial basis function with corresponding coefficient $\theta_j \in \mathbb{R}$. Measurements are generated by sampling $P_o(\xi)$ at 190 nodes, where $\xi = 0.001 \cdot [1, 2, \dots, 100, 110, 120, \dots, 1000]$. These samples are contaminated by multiplicative, normally distributed noise with variance 0.0625, see Fig. 3. The goal is to compute

$$\theta^* = \arg \min_{\theta} \sum_{k=1}^{190} (P_o(\xi_k) - \hat{P}(\xi_k, \theta))^2. \quad (52)$$

B. System identification algorithm

An optimum of (52) is attained if

$$\sum_{k=1}^{190} \frac{\partial}{\partial \theta} (P_o(\xi_k) - \hat{P}(\xi_k, \theta))^2 = 0 \quad (53)$$

holds, which is nonlinear in θ . To solve (53), the iterative approach in [3] is applied. As a result, the polynomial equality

$$\sum_{k=1}^m \frac{\partial g(\xi_k, \theta)}{\partial \theta^T} w_{2k}^T (w_{1k} f(\xi_k, \theta) - h_k) = 0, \quad (54)$$

where

$$f(\xi, \theta^{(i)}) = g(\xi, \theta^{(i)}) = d(\xi, \theta^{(i)}), \quad (55)$$

$$w_{1k} = \frac{P_o(\xi_k)}{d(\xi_k, \theta^{(i-1)})}, \quad (55)$$

$$w_{2k} = \frac{\hat{P}(\xi_k, \theta^{(i-1)})}{d(\xi_k, \theta^{(i-1)})}, \quad (56)$$

$$h_k = \frac{n_o(\xi_k)}{d(\xi_k, \theta^{(i-1)})},$$

is solved iteratively, see also Alg. 43 in App. A. In iteration i , $\hat{P}(\xi, \theta^{(i-1)})$ is available. In the remainder of this section, $i = 1$ is considered. Associated with (54) is the oblique projection

$$(\Psi^T W_2 W_1 \Phi) \theta^{(i)} = \Psi^T W_2 h, \quad (57)$$

where $h = [h_1 \ h_2 \ \dots \ h_m]^T$, see Sect. III-A for details.

C. Exploiting freedom in the selection of polynomial bases

The selection of appropriate polynomial bases is a key step towards the computation of an accurate solution to (57). When using the monomial basis (4), i.e., $\varphi_j(\xi) = \psi_j(\xi) = \phi_{\text{mon},j}(\xi)$, $j = 0, 1, \dots, 6$, the condition number is

$$\kappa(\Phi_{\text{mon}}^T W_2^T W_1 \Phi_{\text{mon}}) = 4.35 \cdot 10^{11}.$$

In the next section, it is shown that the bad conditioning of (57) leads to inaccurate models. This is resolved effectively using the results presented in this paper. Using Alg. 39, the freedom in selection of bases is exploited by constructing polynomial bases $\varphi_j(\xi), \psi_j(\xi)$, $j = 0, 1, \dots, 6$ that are bi-orthonormal with respect to the bi-linear form (21), with w_{1k}, w_{2k} in (55)–(56). Indeed, the main result in Thm. 17 is confirmed, as the use of bi-orthonormal polynomials leads to optimal numerical conditioning of (57):

$$\kappa(\Psi^T W_2^T W_1 \Phi) = 1.00.$$

D. Illustration of the propagation of rounding errors

Next, the consequences of poor numerical conditioning in system identification are shown. To this end, (57) is written as

$$A \theta = b, \quad (58)$$

where $A = (\Psi^T W_2 W_1 \Phi)$ and $b = \Psi^T W_2 h$. Typically, (58) is solved using QR-factorization. To investigate the sensitivity to rounding errors, random perturbations db are added to the righthand side, whereafter resulting perturbations $d\theta$ of the parameter vector are investigated. In accordance with [15, Thm. 5.3.1.], the following bound on the worst-case relative error propagation can be derived:

$$\frac{\|d\theta\|_2}{\|\theta\|_2} \leq \underbrace{\frac{1}{\sigma(A)} \frac{\|A\theta\|_2}{\|\theta\|_2}}_{\text{worst-case amplification for a particular nominal solution } \theta} \cdot \frac{\|db\|_2}{\|b\|_2} \leq \kappa(A) \cdot \frac{\|db\|_2}{\|b\|_2}.$$

When formulating (57) using monomial basis polynomials, $\frac{1}{\sigma(A)} \frac{\|A\theta\|_2}{\|\theta\|_2} = 4.43 \cdot 10^6$. Indeed, in Fig. 4 it is shown that relatively small perturbations, for example due to round-off errors during QR-factorization, might lead to significant perturbations in the parameter vector. This is confirmed in Fig. 5-(a), where a non-negligible difference of the resulting model estimate is obtained by small random perturbations of b . In contrast, when bi-orthonormal polynomial bases are used to formulate (57), then $\kappa(A) = 1$. As a consequence, perturbations in b are not amplified, which leads to a large improvement in model accuracy, see Fig. 5-(b).

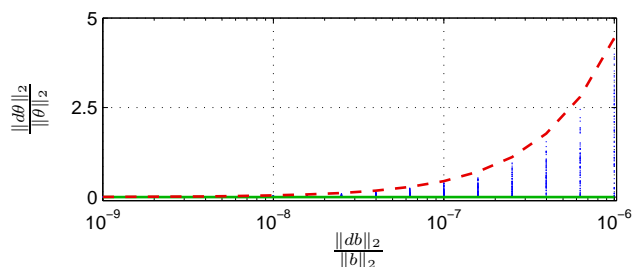
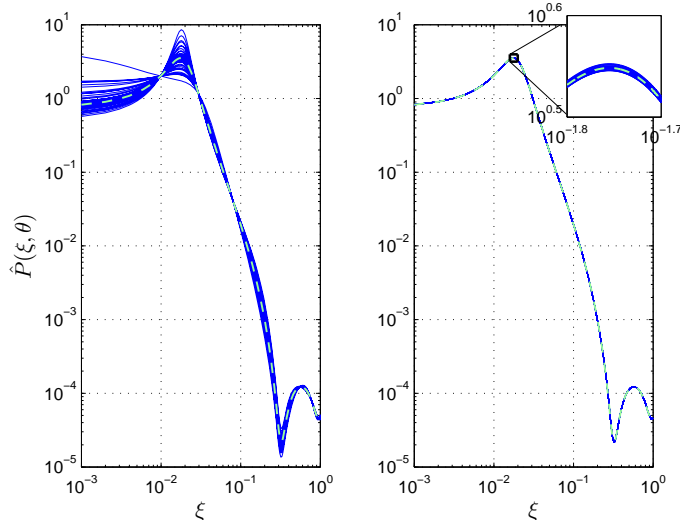


Fig. 4. Monte Carlo simulation of relative error propagation using the monomial basis (blue dots). The worst-case error propagation is indicated with the red, dashed line. The green, solid line indicates the relative error propagation factor 1 that is achieved using bi-orthonormal polynomial bases.



(a) Formulating oblique projection using monomial basis polynomials. (b) Formulating oblique projection in bi-orthonormal polynomial bases.

Fig. 5. Nominal model $\hat{P}(\xi, \theta)$ (dashed) and cloud of models resulting from random perturbations of the righthand side of the oblique projection.

VIII. CONCLUSIONS

In this paper, a polynomial theory for a general class of polynomial equalities that are asymmetric and indefinite is developed. Polynomial bases that are bi-orthonormal with respect to a data-dependent bi-linear form are presented. The optimal approximant of a certain degree is equal to a scaled version of the right basis polynomial of the corresponding degree. As a result, the linear system of equations that results after substitution of the polynomial bases has optimal numerical conditioning, i.e., $\kappa = 1$. The importance of this approach is confirmed by a comparison with traditional approaches, in which the use of one single classical polynomial basis such as the monomial basis, Chebyshev basis, *etc.*, often leads to a severely ill-conditioned linear system of equations, preventing the computation of an accurate solution.

The proposed framework is expected to have many applications in the general field of identification and control, including the nonexhaustive list of applications mentioned in Sect. II-B. As a specific application, the framework is applied to a recent system identification algorithm based on instrumental variables. This particular algorithm is shown to typically lead to poorly conditioned problems. In addition, it is shown that the use of the presented bi-orthonormal polynomials achieves $\kappa = 1$, which cannot be achieved using pre-existing results.

Illustrative simulation examples can be found in [20]. A 16th order successful industrial case study is presented in [22]. Furthermore, an experimental example and comparison with pre-existing approaches is presented in [39]. Finally, recent experiments [40] have shown good results on a 100th order model.

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Two classes of frequency-domain identification algorithms are presented, which connect to polynomial approximation. Consider a true system $P_o(\xi)$, where ξ represents the s-domain or z-domain. Let $\hat{P}(\xi, \theta)$ be the real-rational model

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

with $n(\xi, \theta), d(\xi, \theta) \in \mathbb{R}[\xi]$. In weighted least-squares identification, the goal is, for a given weighting function $W(\xi)$, to determine the optimal model parameters θ by minimizing

$$\mathcal{V}(\theta) = \sum_{k=1}^m |\varepsilon(\xi_k, \theta)|^2 := \sum_{k=1}^m |W(\xi_k)(P_o(\xi_k) - \hat{P}(\xi_k, \theta))|^2. \quad (59)$$

Remark 41. To ensure that the minimum to $\mathcal{V}(\theta)$ in (59) is a real-valued parameter vector θ , the nodes ξ_k , $k = 1, \dots, m$ should be a set of complex-conjugate pairs, cf. [36, Sect. 5]. Thus, both positive and negative frequencies should be considered.

Since (59) is non-linear in real-valued parameters θ , it may have several local minima, which are attained when $\frac{\partial \mathcal{V}(\theta)}{\partial \theta^T} = 0$.

Lemma 42. A (local) optimum of $\mathcal{V}(\theta)$ in (59) is attained if

$$\sum_{k=1}^m \left[\frac{-\partial \hat{P}(\xi_k, \theta)}{\partial \theta^T} \right]^H W^H(\xi_k) W(\xi_k) (P_o(\xi_k) - \hat{P}(\xi_k, \theta)) = 0. \quad (60)$$

Proof: Define $\zeta(\xi_k, \theta) := \frac{\partial \varepsilon(\xi_k, \theta)}{\partial \theta^T} = -W(\xi_k) \frac{\partial \hat{P}(\xi_k, \theta)}{\partial \theta^T}$. The result is obtained by observing that $\frac{\partial \mathcal{V}(\theta)}{\partial \theta^T} = 0$ is equivalent with $\sum_{k=1}^m \zeta^H(\xi_k, \theta) \varepsilon(\xi_k, \theta) = 0$. ■

To solve nonlinear equation (60) in θ , [3] proposes an iterative algorithm where in iteration i use is made of an estimate $\hat{P}(\xi, \theta^{(i-1)})$ from a previous iteration.

Algorithm 43 (Frequency-domain IV identification).

Let $\hat{P}(\xi, \theta^{(i-1)})$ be given. In iteration i , the polynomial approximation problem (1) is solved, where

$$f(\xi, \theta) = g(\xi, \theta) = [d(\xi, \theta^{(i)}) \quad n(\xi, \theta^{(i)})]^T, \quad (61)$$

and

$$w_{1k} = \frac{W(\xi_k)}{d(\xi_k, \theta^{(i-1)})} [P_o(\xi_k) \quad -1], \quad (62)$$

$$w_{2k} = \frac{W(\xi_k)}{d(\xi_k, \theta^{(i-1)})} [\hat{P}(\xi, \theta^{(i-1)}) \quad -1].$$

Indeed, then (1) approximates (60), as is verified by solving

$$\begin{aligned} -\frac{\partial \hat{P}(\xi, \theta)}{\partial \theta^T} &= \frac{\partial}{\partial \theta^T} \left(\begin{bmatrix} 0 & -1 \\ d(\xi, \theta) & n(\xi, \theta) \end{bmatrix} \right) \\ &= \frac{\partial d(\xi, \theta)}{\partial \theta^T} \begin{bmatrix} 0 & -1 \\ d(\xi, \theta) & n(\xi, \theta) \end{bmatrix} + \frac{-1}{d(\xi, \theta)} \frac{\partial n(\xi, \theta)}{\partial \theta^T} \\ &= \frac{1}{d(\xi, \theta)} [\hat{P}(\xi, \theta) \quad -1] \frac{\partial}{\partial \theta^T} \left(\begin{bmatrix} d(\xi, \theta) \\ n(\xi, \theta) \end{bmatrix} \right), \end{aligned}$$

in which $\hat{P}(\xi, \theta^{(i-1)})$ and $d(\xi, \theta^{(i-1)})$ are then substituted using the previous iteration $i-1$, and subsequently rewriting

$$\varepsilon(\xi, \theta) = \frac{W(\xi)}{d(\xi, \theta)} \begin{bmatrix} P_o(\xi) & 1 \end{bmatrix} \begin{bmatrix} d(\xi, \theta) \\ n(\xi, \theta) \end{bmatrix}, \quad (63)$$

in which $d(\xi, \theta^{(i-1)})$ is to be substituted. ■

An alternative algorithm is often encountered in literature. It aims to solve (59) using linear least-squares optimization.

Algorithm 44 (Sanathanan-Koerner iteration). [34]

Let $d(\xi, \theta^{(i-1)})$ be given. In iteration i , polynomial approximation problem (12) is solved, with $f(\xi, \theta)$, w_{1k} in (61)–(62). By using $\varepsilon(\xi, \theta)$ in (63), in which $d(\xi, \theta^{(i-1)})$ is substituted, it can be verified that (12) approximates (59).

APPENDIX B PROOFS OF AUXILIARY RESULTS

Proof of Theorem 21 First, *necessity* is proven. Consider the decomposition

$$W_2^T W_1 = W_{\text{sym}} + W_{\text{skew}},$$

where

$$\begin{aligned} W_{\text{sym}} &= \frac{1}{2} (W_2^T W_1 + W_1^T W_2), \\ W_{\text{skew}} &= \frac{1}{2} (W_2^T W_1 - W_1^T W_2). \end{aligned}$$

Because the transpose of (28) yields $\Phi^T W_1^T W_2 \Phi = D$, it follows that (28) is equivalent to:

$$\Phi^T W_{\text{sym}} \Phi = D, \quad (64a)$$

$$\Phi^T W_{\text{skew}} \Phi = 0. \quad (64b)$$

Since any generic polynomial basis $\varphi_j(\xi)$, $j = 0, 1, \dots, n-1$ is related to the monomial basis $\phi_{\text{mon},k}(\xi)$ in (4) through

$$\varphi_j(\xi) = \sum_{k=0}^j s_{jk} \phi_{\text{mon},k}(\xi),$$

Φ in (14) can be written as

$$\Phi = V_q S, \quad (65)$$

where

$$V_q := \begin{bmatrix} I_q & \xi_1 I_q & \dots & \xi_1^{n-1} I_q \\ I_q & \xi_2 I_q & \dots & \xi_2^{n-1} I_q \\ \vdots & \vdots & \ddots & \vdots \\ I_q & \xi_m I_q & \dots & \xi_m^{n-1} I_q \end{bmatrix}, \quad S := \begin{bmatrix} s_{00} & s_{10} & \dots & s_{n-1,0} \\ & s_{11} & \dots & s_{n-1,1} \\ & & \ddots & \vdots \\ & & & s_{n-1,n-1} \end{bmatrix}.$$

Here, $V_q \in \mathbb{R}^{mq \times nq}$ and $S \in \mathbb{R}^{nq \times nq}$, where S is full rank since s_{jj} , $j = 0, 1, \dots, n-1$ are invertible by assumption, cf. Sect. II-A. Consequently, it follows after inserting (65) that (64b) requires

$$V_q^T W_{\text{skew}} V_q = 0,$$

which only holds if $S_{ij} = 0 \forall i, j = 0, 1, \dots, n-1$.

Next, *sufficiency* is proven. As shown above, if $S_{ij} = 0 \forall i, j = 0, 1, \dots, n-1$, then (64b) holds. It remains to select $\varphi_j(\xi)$, $j = 0, 1, \dots, n-1$ such that (64a) holds. Inserting (65) yields

$$S^T V_q^T W_{\text{sym}} V_q S = D. \quad (66)$$

The matrix $V_q^T W_{\text{sym}} V_q$ is symmetric and is of full rank for well-posed problems. As a consequence, by selecting

$S = L^{-T}$, where L follows from the LDU-decomposition for Hermitian matrices [15, Sect. 4.1, 4.4]

$$V_q^T W_{\text{sym}} V_q = L D L^T,$$

(66) is satisfied, hence, (28) holds. ■

Proof of Lemma 31 Since $\tilde{L}^T \tilde{K} = I$ implies that $\tilde{L} = \tilde{K}^{-T}$, it holds that:

$$(\tilde{L}^T X \tilde{K})^j = \underbrace{(\tilde{L}^T X \tilde{K})(\tilde{L}^T X \tilde{K}) \dots (\tilde{L}^T X \tilde{K})}_{j \text{ terms}} = \tilde{L}^T X^j \tilde{K}.$$

Now define $H_1 := \tilde{L}^T X \tilde{K}$, which is used to formulate:

$$\tilde{L}^T [\tilde{K} \ X \tilde{K} \ \dots \ X^{n-1} \tilde{K}] = [I \ H_1 \ \dots \ H_1^{n-1}].$$

Post-multiplying both sides with $I_n \otimes e_1$, where $e_1 = [1 \ 0 \ \dots \ 0]^T \in \mathbb{R}^{n \times 1}$ is the first standard basis vector and \otimes denotes the Kronecker product, yields:

$$\tilde{L}^T [\tilde{k}_1 \ X \tilde{k}_1 \ \dots \ X^{n-1} \tilde{k}_1] = [e_1 \ H_1 e_1 \ \dots \ H_1^{n-1} e_1]. \quad (67)$$

Using (42), the left-hand side of (67) can be rewritten as:

$$\frac{1}{\sqrt{|l_1^T k_1|}} \tilde{L}^T [k_1 \ X k_1 \ \dots \ X^{n-1} k_1] = \frac{1}{\sqrt{|l_1^T k_1|}} \tilde{L}^T K.$$

Since $\tilde{L}^T \tilde{K} = I$, pre-multiplication of (41) with \tilde{L}^T yields $\tilde{L}^T K = S^{-1}$. By combining this result with (36), it follows that (67) is equivalent to:

$$\frac{1}{\sqrt{|l_1^T k_1|}} S^{-1} = [e_1 \ \mathcal{T} e_1 \ \dots \ \mathcal{T}^{n-1} e_1],$$

which is an upper triangular matrix since S is upper triangular. This implies that H_1 is *upper Hessenberg*. ■

Proof of Theorem 33 To start with, equality of the first row and column of (44) is proven. It follows from (42)–(43) that

$$\underline{W}_1 = \tilde{k}_1 \sqrt{|l_1^T k_1|},$$

$$\text{sign}(W_2^T \underline{W}_1) \cdot \underline{W}_2 = \tilde{l}_1 \sqrt{|l_1^T k_1|}.$$

Hence, by virtue of bi-orthonormality of \tilde{K} and \tilde{L} :

$$\tilde{L}^T \underline{W}_1 = \sqrt{|l_1^T k_1|} \tilde{L}^T \tilde{k}_1 = \begin{bmatrix} \gamma_0 \\ 0_{m-1,1} \end{bmatrix},$$

$$\underline{W}_2^T \tilde{K} = \text{sign}(l_1^T k_1) \cdot \sqrt{|l_1^T k_1|} \tilde{l}_1^T \tilde{K} = [\beta_0 \ 0_{1,m-1}],$$

where $\gamma_0 = \sqrt{|l_1^T k_1|}$ and $\beta_0 = \text{sign}(l_1^T k_1) \sqrt{|l_1^T k_1|}$, hence, $|\beta_0| = \gamma_0$. It remains to show that $\tilde{L}^T X \tilde{K}$ is a tri-diagonal matrix. Observe that, since $\xi_k, w_{1k}, w_{2k} \in \mathbb{R}$, $k = 1, \dots, m$,

$$H_2 = \tilde{K}^T X \tilde{L} = (\tilde{L}^T X \tilde{K})^T = H_1^T.$$

where use is made of Lemma 31 and Lemma 32. Thus, the matrix $\tilde{L}^T X \tilde{K}$ is both upper and lower Hessenberg, hence, tri-diagonal, which proves the theorem. ■

Proof of Lemma 35 Since $\tilde{L}^T \tilde{K} = I$, or, equivalently, $\tilde{L}^T = \tilde{K}^{-1}$, the lower right component of the eigenvalue decomposition (44) induces the following equations:

$$X \tilde{K} = \tilde{K} \mathcal{T}, \quad (68)$$

$$X \tilde{L} = \tilde{L} \mathcal{T}^T. \quad (69)$$

Evaluating (68)–(69) per column, while taking into account the structure of \mathcal{T} in (45), yields the following three-term-recursions for the columns of \tilde{K} and \tilde{L} :

$$\begin{aligned} X \tilde{k}_j &= \beta_{j-1} \tilde{k}_{j-1} + \alpha_j \tilde{k}_j + \gamma_j \tilde{k}_{j+1}, \\ X \tilde{l}_j &= \gamma_{j-1} \tilde{l}_{j-1} + \alpha_j \tilde{l}_j + \beta_j \tilde{l}_{j+1}. \end{aligned}$$

Rearranging terms yields (46)–(47). ■

Proof of Theorem 36 Select the 0th order polynomials $\varphi_0(\xi)$ and $\psi_0(\xi)$:

$$\begin{aligned} \varphi_0(\xi) &= 1 / \sqrt{|l_1^T k_1|} = 1 / \sqrt{|W_2^T W_1|}, \quad (70) \\ \psi_0(\xi) &= \text{sign}(l_1^T k_1) / \sqrt{|l_1^T k_1|} \\ &= \text{sign}(W_2^T W_1) / \sqrt{|W_2^T W_1|}. \quad (71) \end{aligned}$$

Let Φ_j, Ψ_j denote the j^{th} column of Φ, Ψ in (14)–(15). Then, using (16) and (42)–(43) it follows that

$$\begin{aligned} W_1 \Phi_1 &= \tilde{k}_1, \\ W_2 \Psi_1 &= \tilde{l}_1. \end{aligned}$$

Consequently,

$$[\varphi_0(\xi), \psi_0(\xi)] = \Psi_1^T W_2^T W_1 \Phi_1 = \tilde{l}_1^T \tilde{k}_1 = 1.$$

Now, let $\varphi_j(\xi), \psi_j(\xi), j = 1, 2, \dots$ be constructed using the recursion relations (48)–(49), with $\varphi_{-1} := 0, \psi_{-1} := 0$ and $\varphi_0(\xi), \psi_0(\xi)$ as given in (70)–(71). As a result, by virtue of the *vector*-recursion relations (46)–(47) in Lemma 35,

$$\begin{aligned} W_1 \Phi_{j+1} &= \tilde{k}_{j+1}, \\ W_2 \Psi_{j+1} &= \tilde{l}_{j+1}. \end{aligned}$$

Finally, since

$$[\varphi_i(\xi), \psi_j(\xi)] = \Psi_{j+1}^T W_2^T W_1 \Phi_{i+1} = \tilde{l}_{j+1}^T \tilde{k}_{i+1} = \delta_{ij},$$

bi-orthonormality of the polynomials $\varphi_i(\xi)$ and $\psi_j(\xi), i, j = 0, 1, \dots, n-1$, follows from bi-orthonormality of the Krylov bases \tilde{K} and \tilde{L} . ■

Proof of Lemma 37 The proof follows by induction. The polynomials $\varphi_0(\xi)$ and $\psi_0(\xi)$, see (70)–(71), are chosen such that $\psi_0(\xi) = \pm \varphi_0(\xi)$, where $\varphi_0 > 0$. Hence,

$$\psi_0(\xi) = \text{sign}(\psi_0) \cdot \varphi_0(\xi).$$

From (48)–(49), it follows that

$$\begin{aligned} \varphi_1(\xi) &= \frac{1}{\gamma_1} (\xi - \alpha_1) \varphi_0(\xi), \\ \psi_1(\xi) &= \frac{1}{\beta_1} (\xi - \alpha_1) \psi_0(\xi). \end{aligned}$$

Since in Lemma 37, $\beta_k = \pm \gamma_k, \gamma_k > 0$ holds by assumption,

$$\beta_k = \text{sign}(\beta_k) \gamma_k. \quad (72)$$

Thus,

$$\psi_1(\xi) = \text{sign}(\psi_0) \text{sign}(\beta_1) \cdot \varphi_1(\xi).$$

As a result, $\psi_1(\xi) = s_1 \cdot \varphi_1(\xi)$ where $s_1 := \text{sign}(\psi_0) \text{sign}(\beta_1)$. In general, let

$$\psi_i(\xi) = s_i \cdot \varphi_i(\xi), \quad (73)$$

$$s_i := \text{sign}(\psi_0) \text{sign}(\beta_1) \cdots \text{sign}(\beta_i) \quad (74)$$

hold for $i = k-1, i = k-2$. The proof of Lemma 37 follows by showing that this relation also holds for $i = k$. In particular, observe that (48)–(49) equal

$$\begin{aligned} \varphi_k(\xi) &= \frac{1}{\gamma_k} ((\xi - \alpha_k) \varphi_{k-1}(\xi) - \beta_{k-1} \varphi_{k-2}(\xi)), \\ \psi_k(\xi) &= \frac{1}{\beta_k} ((\xi - \alpha_k) \psi_{k-1}(\xi) - \gamma_{k-1} \psi_{k-2}(\xi)) \\ &= \text{sign}(\beta_k) \frac{1}{\gamma_k} ((\xi - \alpha_k) s_{k-1} \varphi_{k-1}(\xi) - \dots \quad (75) \\ &\quad \gamma_{k-1} s_{k-2} \varphi_{k-2}(\xi)) \\ &= \text{sign}(\beta_k) \frac{1}{\gamma_k} (s_{k-1} \cdot (\xi - \alpha_k) \varphi_{k-1}(\xi) - \dots \quad (76) \\ &\quad s_{k-1} \cdot \beta_{k-1} \varphi_{k-2}(\xi)), \end{aligned}$$

where in (75) use is made of (72) and (73), and in (76) use is made of (72) and (74). Finally, by applying (74) to (76) again, it follows that $\psi_k(\xi) = s_k \varphi_k(\xi)$, i.e., (73) holds for $i = k$ indeed. This proves that (51) holds. ■

Proof of Theorem 38 By virtue of Lemma 37, (51) holds. As an immediate consequence, bi-orthonormality of the polynomials $\varphi_i(\xi)$ and $\psi_j(\xi)$ as defined in Def. 15 is equivalent with orthonormality with respect to an indefinite inner product, cf. Def. 22, for the *individual* polynomial bases $\varphi_i(\xi)$ as well as $\psi_j(\xi)$. ■



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