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Vector versions of Prony's algorithm and vector-valued rational approximations

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Abstract

Given the scalar sequence $\{f_m\}_{m=0}^{\infty}$ that satisfies

$$f_m = \sum_{i=1}^{k} a_i \zeta_i^m, \quad m = 0, 1, \ldots,$$

where $a_i, \zeta_i \in \mathbb{C}$ and ζ_i are distinct, the algorithm of Prony concerns the determination of the a_i and the ζ_i from a finite number of the f_m. This algorithm is also related to Padé approximants from the infinite power series $\sum_{j=0}^{\infty} f_j z^j$. In this work, we discuss ways of extending Prony's algorithm to sequences of vectors $\{\boldsymbol{f}_m\}_{m=0}^{\infty}$ in $\mathbb{C}^N$ that satisfy

$$\boldsymbol{f}_m = \sum_{i=1}^{k} \boldsymbol{a}_i \zeta_i^m, \quad m = 0, 1, \ldots,$$

where $\boldsymbol{a}_i \in \mathbb{C}^N$ and $\zeta_i \in \mathbb{C}$. Two distinct problems arise depending on whether the vectors $\boldsymbol{a}_i$ are linearly independent or not. We consider different approaches that enable us to determine the $\boldsymbol{a}_i$ and ζ_i for these two problems, and develop suitable methods. We concentrate especially on extensions that take into account the possibility of the components of the $\boldsymbol{a}_i$ being coupled. One of the applications we consider concerns the case in which

$$\boldsymbol{f}_m = \sum_{i=1}^{r} \boldsymbol{a}_i \zeta_i^m, \quad m = 0, 1, \ldots, \quad r \text{ large},$$

and we would like to approximate/determine of a number of the pairs $(\zeta_i, \boldsymbol{a}_i)$ for which $|\zeta_i|$ are largest. We present the related theory and provide numerical examples

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that confirm this theory. This application can be extended to the more general case in which

$$\boldsymbol{f}_m = \sum_{i=1}^{r} \boldsymbol{p}_i(m)\zeta_i^m, \quad m = 0, 1, \ldots,$$

where $\boldsymbol{p}_i(m) \in \mathbb{C}^N$ are some (vector-valued) polynomials in m, and $\zeta_i \in \mathbb{C}$ are distinct. Finally, the methods suggested here can be extended to vector sequences in infinite dimensional spaces in a straightforward manner.

Keywords Prony algorithm · Padé approximants · Vector-valued rational approximations

Mathematics subject classification (2010) 65F20 · 65F50 · 65H10

1 Introduction

Consider a function $f(t)$ that is a sum of exponential functions given as

$$f(t) = \sum_{i=1}^{k} \gamma_i \exp(\eta_i t), \quad \gamma_i \neq 0, \quad \eta_i \text{ distinct.} \tag{1.1}$$

We wish to determine the γ_i and η_i. To achieve this, we compute $f(t)$ at the equidistant points $t_m = t_0 + mh$, $m = 0, 1, \ldots,$ with some fixed $h > 0$. This gives rise to the system of equations

$$f(t_m) = \sum_{i=1}^{k} \gamma_i \exp(\eta_i t_m), \quad m = 0, 1, \ldots. \tag{1.2}$$

Letting $f_m = f(t_m)$, $a_i = \gamma_i \exp(\eta_i t_0)$, and $\zeta_i = \exp(\eta_i h)$, these equations become

$$f_m = \sum_{i=1}^{k} a_i \zeta_i^m, \quad m = 0, 1, \ldots. \tag{1.3}$$

Clearly, $a_i, \zeta_i \in \mathbb{C}$, $i = 1, \ldots, k$, are independent of m, and ζ_i are distinct. We would like to determine the a_i and the ζ_i from the f_m, from which, we will be able obtain the γ_i and η_i in general. Since there are $2k$ unknowns in this problem, we need $2k$ equations, and these can be taken from (1.3). Let us choose those equations with $m = 0, 1, \ldots, 2k-1$, for example. The well-known algorithm of Prony [15] solves these equations and obtains the a_i and ζ_i as follows:

1. Solve the $k \times k$ linear system

$$\sum_{j=0}^{k-1} f_{m+j} u_j = -f_{m+k}, \quad m = 0, 1, \ldots, k-1, \tag{1.4}$$

   for $u_0, u_1, \ldots, u_{k-1}$, and set $u_k = 1$.
2. Obtain $\zeta_1, \ldots, \zeta_k$ as the roots of the polynomial equation $\sum_{j=0}^{k} u_j \zeta^j = 0$.

3. With $\zeta_1, \ldots, \zeta_k$ available, solve the $k \times k$ linear system

$$\sum_{i=1}^{k} a_i \zeta_i^m = f_m, \quad m = 0, 1, \ldots, k-1, \tag{1.5}$$

for $a_1, \ldots, a_k$. Written in full, this system reads

$$\boldsymbol{V}^T \boldsymbol{a} = \boldsymbol{f}, \tag{1.6}$$

where

$$\boldsymbol{V} = \begin{bmatrix} 1 & \zeta_1 & \cdots & \zeta_1^{k-1} \\ 1 & \zeta_2 & \cdots & \zeta_2^{k-1} \\ \vdots & \vdots & & \vdots \\ 1 & \zeta_k & \cdots & \zeta_k^{k-1} \end{bmatrix}, \quad \boldsymbol{a} = [a_1, a_2, \ldots, a_k]^T, \quad \boldsymbol{f} = [f_0, f_1, \ldots, f_{k-1}]^T. \tag{1.7}$$

Here $\boldsymbol{V}$ is a Vandermonde matrix. (Note that $\boldsymbol{V}$ is nonsingular since the ζ_i are distinct.)

The equations (1.4) that provide the u_j can be obtained as follows: Starting with

$$u(\zeta) = \prod_{i=1}^{k} (\zeta - \zeta_i) = \sum_{j=0}^{k} u_j \zeta^j, \quad u_k = 1,$$

and invoking (1.3), we have, for $m = 0, 1, \ldots,$

$$\begin{aligned} \sum_{j=0}^{k} u_j f_{m+j} &= \sum_{j=0}^{k} u_j \sum_{i=1}^{k} a_i \zeta_i^{m+j} \\ &= \sum_{i=1}^{k} a_i \zeta_i^m \sum_{j=0}^{k} u_j \zeta_i^j \\ &= \sum_{i=1}^{k} a_i \zeta_i^m u(\zeta_i) \\ &= 0. \end{aligned}$$

The a_i can also be determined—without having to solve the system in (1.6) numerically—by resorting to the connection between Prony's algorithm with the Padé table. We present a detailed discussion of this issue in the next section.

In Section 3, we introduce four procedures that extend Prony's algorithm to sequences of *vectors* $\{\boldsymbol{f}_m\}_{m=0}^{\infty}$ [as opposed to sequences of *scalars* $\{f_m\}_{m=0}^{\infty}$ in (1.3)], and consider the numerical implementations of these procedures under different circumstances. In Section 4, we discuss the connection of these procedures with some vector-valued rational approximation procedures and discuss an additional application that is closely related to, and yet outside the realm of, Prony's algorithm. Specifically, the problem we are interested in involves the determination of a number of those ζ_j that have largest modulus. The approach of Section 2 involving rational approximations is used throughout. In Section 6, we provide numerical examples that illustrate the use of the approach of Section 4 and that confirm the theory presented there. The relation of Prony's algorithm to Padé approximants was discussed originally by Weiss and McDonough [26]. The results of [26] were generalized by Sidi [18, 19] to cover the cases in which

$$f_m = \sum_{i=1}^{s} a_i(m)\zeta_i^m, \quad m = 0, 1, \ldots, ; \quad a_i(m) \text{ polynomials in } m,$$

which occur when the polynomial $u(\zeta)$ has at least one multiple root. Padé approximants continue to play a crucial role in these generalizations too. For Padé approximants, see Baker and Graves-Morris [1] and Gilewicz [7]. For a very effective procedure for computing Padé approximants, see Trefethen [25, Chapter 27]. For a detailed summary that includes some of the results of [18] and [19], see also Sidi [22, Chapter 17].

The algorithm of Prony and its various generalizations are discussed and applied in a variety of contexts and in numerous areas. It is known (see [18]) that Prony's algorithm does not always have a solution when the set $\{f_m\}_{m=0}^{2k-1}$ is arbitrary, that is, when the f_m are not necessarily as in (1.3). This implies that the problem of determining the parameters ζ_i, a_i is not always stable numerically. To circumvent this problem, Prony's algorithm has been modified in several ways, giving rise to some very effective methods that cope successfully with the problem of numerical instability. Among these, we mention the multiple signal classification method (MUSIC) of Schmidt [17], estimation of signal parameters via rotational invariance techniques (ESPRIT) of Roy and Kailath [16], fast ESPRIT algorithms of Potts and Tasche [14], the matrix pencil method of Hua and Sarkar [10] and Golub, Milanfar, and Varah [8], the annihilating vector method of Dragotti, Vetterli, and Blu [6], and the approximate Prony method of Potts and Tasche [13]. Recently, Prony's algorithm has also been extended to the solution of sparse multivariate problems in the papers by Ben-Or and Tiwari [2], Cuyt and Lee [4], and Cuyt, Lee, and Yang [5], for example. Another interesting modification of Prony's algorithm has been developed for sparse eigenfunction expansions in the works of Peter and Plonka [11] and Plonka and Tasche [12].

2 Padé approximants and Prony's algorithm

Let $f(z) = \sum_{j=0}^{\infty} f_j z^j$ be a formal power series. When it exists, the $[m/n]$ Padé approximant from $f(z)$, which we denote $f_{m,n}(z)$, is defined as follows:

$$f_{m,n}(z) = \frac{P(z)}{Q(z)}; \quad P \in \pi_m, \quad Q \in \pi_n, \quad Q(0) = 1, \tag{2.1}$$

$$f(z) - f_{m,n}(z) = O(z^{m+n+1}) \quad \text{as } z \to 0. \tag{2.2}$$

It is easy to realize that (2.2) implies

$$Q(z)f(z) - P(z) = O(z^{m+n+1}) \quad \text{as } z \to 0. \tag{2.3}$$

Letting $P(z)=\sum_{i=0}^{m}p_iz^i$ and $Q(z)=\sum_{j=0}^{n}q_jz^j$, $q_0=1$, it follows from (2.3) that the p_i and q_i satisfy the $m+n+1$ linear equations

$$\sum_{j=0}^{\min(i,n)} f_{i-j}q_j = p_i, \quad i=0,1,\ldots,m, \tag{2.4}$$

$$\sum_{j=0}^{\min(i,n)} f_{i-j}q_j = 0, \quad i=m+1,\ldots,m+n, \tag{2.5}$$

and that

$$f_{m,n}(z)=\frac{\sum_{j=0}^{n}q_jz^js_{m-j}(z)}{\sum_{j=0}^{n}q_jz^j}, \tag{2.6}$$

where

$$s_r(z)=\sum_{j=0}^{r}f_jz^j, \quad r=0,1,\ldots; \quad s_r(z)\equiv 0 \text{ if } r<0. \tag{2.7}$$

It is known that, if it exists, $f_{m,n}(z)$ is unique. It is also known that if $f(z)$ is a rational function (having no pole at $z=0$) with degree of numerator and degree of denominator (after complete reduction) being m and n, respectively, then $f_{m,n}(z)\equiv f(z)$; that is, Padé approximants reproduce rational functions from whose Maclaurin series they are derived.

The algorithm of Prony described in the preceding section is related to $f_{k-1,k}(z)$ from $f(z)=\sum_{j=0}^{\infty}f_jz^j$, with the f_j as in (1.3), as follows: First, note that $f(z)$ is a rational function with degree of numerator equal to $k-1$ at most and degree of denominator equal to k:

$$f(z)=\sum_{j=0}^{\infty}f_jz^j=\sum_{j=0}^{\infty}\left(\sum_{i=1}^{k}a_i\zeta_i^j\right)z^j=\sum_{i=1}^{k}a_i\sum_{j=0}^{\infty}(\zeta_iz)^j=\sum_{i=1}^{k}\frac{a_i}{1-\zeta_iz}. \tag{2.8}$$

Therefore, $f_{k-1,k}(z)\equiv f(z)$. Let the partial fraction decomposition of $f_{k-1,k}(z)$ be as in

$$f_{k-1,k}(z)=\frac{P(z)}{Q(z)}=\sum_{i=1}^{k}\frac{w_i}{z-z_i}, \tag{2.9}$$

where z_i are the zeros of the denominator polynomial $Q(z)$. Then the a_i and ζ_i in Prony's algorithm are given as

$$\zeta_i=z_i^{-1}, \quad a_i=-w_iz_i^{-1}, \quad i=1,\ldots,k. \tag{2.10}$$

It is easy to realize that the polynomial $u(\zeta)$ in Prony's algorithm and the denominator polynomial $Q(z)$ of $f_{k-1,k}(z)$ are related via

$$u(\zeta)=\zeta^kQ(\zeta^{-1}) \quad \Leftrightarrow \quad u_j=q_{k-j}, \quad j=0,1,\ldots,k. \tag{2.11}$$

As a result, we do not need to solve the linear system in (1.6) to obtain the a_i because the w_i in (2.10) can be computed from

$$w_i = \operatorname{Res} f_{k-1,k}(z)\Big|_{z=z_i} = \frac{P(z)}{Q'(z)}\bigg|_{z=z_i} = \frac{\sum_{j=0}^{k} q_j z^j s_{k-1-j}(z)}{\sum_{j=0}^{k} j q_j z^{j-1}}\Bigg|_{z=z_i}, \quad i=1,\dots,k. \tag{2.12}$$

When expressed in terms of the u_j instead of the q_j, this can also be written as

$$w_i = \frac{\sum_{j=0}^{k} u_j z^{k-j} s_{j-1}(z)}{\sum_{j=0}^{k}(k-j)u_j z^{k-j-1}}\Bigg|_{z=z_i}, \quad i=1,\dots,k. \tag{2.13}$$

3 Extensions of Prony's algorithm to vector sequences

3.1 Introduction and a naive approach

Let $\{\boldsymbol{f}_m\}_{m=0}^{\infty}$ be a given sequence of vectors in $\mathbb{C}^N$ such that

$$\boldsymbol{f}_m = \sum_{i=1}^{k} \boldsymbol{a}_i \zeta_i^m, \quad m = 0, 1, \dots, \tag{3.1}$$

where $\boldsymbol{a}_i \in \mathbb{C}^N \setminus \{\boldsymbol{0}\}$ and $\zeta_i \in \mathbb{C}$, $i = 1, \dots, k$, are independent of m, and ζ_i are distinct. Here, N can be arbitrarily large. We would like to determine the $\boldsymbol{a}_i$ and the ζ_i via our knowledge of the $\boldsymbol{f}_m$.

Before proceeding to the solution of this problem, we present an application that gives rise to a vector sequence of the form described in (3.1). Let $f(\boldsymbol{x}, t)$ be a physical quantity that is known, or conjectured, to be of the form $f(\boldsymbol{x}, t) = \sum_{i=1}^{k} \gamma_i(\boldsymbol{x}) \exp(\eta_i t)$. Here $\boldsymbol{x}$ and t may denote, for example, location and time, respectively. The function $f(\boldsymbol{x}, t)$ is being measured at different locations $\boldsymbol{x}_r$, $r = 1, \dots, N$, and at different times $t_m = t_0 + mh$, $m = 0, 1, \dots,$ for some $h > 0$. Thus,

$$f(\boldsymbol{x}_r, t_m) = \sum_{i=1}^{k} \gamma_i(\boldsymbol{x}_r) \exp(\eta_i t_m), \quad m = 0, 1, \dots,$$

which, upon letting

$$\boldsymbol{f}_m = [f(\boldsymbol{x}_1, t_m), \dots, f(\boldsymbol{x}_N, t_m)]^T$$

and

$$\boldsymbol{a}_i = [\gamma_i(\boldsymbol{x}_1) \exp(\eta_i t_0), \dots, \gamma_i(\boldsymbol{x}_N) \exp(\eta_i t_0)]^T, \quad \zeta_i = \exp(\eta_i h), \quad i = 1, \dots, k,$$

results in (3.1).

It is clear that we can apply Prony's algorithm to the sequence $\{\boldsymbol{f}_m\}_{m=0}^{\infty}$ componentwise. That is, we can apply it separately to each of the scalar sequences $\{f_{i,m}\}_{m=0}^{\infty}$, $i = 1, \dots, N$. Given the fact that the $\boldsymbol{f}_m$ satisfy (3.1), the ζ_i produced for each i are the same. Clearly, for this implementation, we need $2k$ of the $\boldsymbol{f}_m$, precisely as in the scalar case.

This approach has a serious drawback, however. In the presence of errors (noise and floating-point errors and others) in the given $\boldsymbol{f}_m$, the polynomials $u(\zeta)$ and hence their zeros ζ_i produced from each application of the (scalar) Prony algorithm will be different. In addition, the possible coupling of the different components $f_{i,m}$, $i = 1, \ldots, N$, of the vectors $\boldsymbol{f}_m$ is lost in the process. Retaining this coupling when it exists may have a beneficial effect, and we aim at this below.

Throughout the remainder of this work, we use lowercase italic letters to denote vectors and uppercase italic letters to denote matrices. In addition, we use the standard Euclidean inner product $(\cdot\,,\cdot)$ and the vector norm $\|\cdot\|$ induced by it; thus $(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{x}^*\boldsymbol{y}$ and $\|\boldsymbol{x}\| = \sqrt{\boldsymbol{x}^*\boldsymbol{x}}$.

3.2 Vectorized algorithms for determining $u(\zeta) = \sum_{j=0}^{k} u_j \zeta^j$

By applying Prony's algorithm to the sequence $\{\boldsymbol{f}_m\}_{m=0}^{\infty}$ componentwise, we realize that $\zeta_1, \ldots, \zeta_k$ are the roots of the polynomial $u(\zeta) = \sum_{j=0}^{k} u_j \zeta^j$, whose coefficients satisfy the vector equations

$$\sum_{j=0}^{k} u_j \boldsymbol{f}_{m+j} = \boldsymbol{0}, \quad m = 0, 1, \ldots. \tag{3.2}$$

Clearly, for each m, we have N scalar homogeneous linear equations satisfied by the u_j. We aim at solving these equations by normalizing the u_j suitably. After determining the u_j, we solve $u(\zeta) = 0$ and obtain $\zeta_1, \ldots, \zeta_k$, as before. With the ζ_i available, we next determine the $\boldsymbol{a}_i$ as the solution to (3.1).

We now want to propose ways—different than that resulting from the naive approach above—of determining a polynomial $u(\zeta)$ that is good for *all* of the sequences $\{f_{i,m}\}_{m=0}^{\infty}$, such that we have only one set of $\zeta_1, \ldots, \zeta_k$ for all N components $f_{i,m}$, $i = 1, \ldots, N$, of the $\boldsymbol{f}_m$, and the coupling of these components is preserved. This can be done in different ways.

We differentiate between two cases: (i) $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_k$ are linearly independent, (ii) $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_k$ are linearly dependent.

3.2.1 The case $a_1, \ldots, a_k$ are linearly independent

When the vectors $\boldsymbol{a}_i$ are linearly independent, which can occur only when $k \le N$, it suffices to consider *only one* of the equations in (3.2). Let us choose that with $m = 0$. We thus solve the $N \times (k+1)$ homogeneous linear system

$$\sum_{j=0}^{k} u_j \boldsymbol{f}_j = \boldsymbol{0} \quad \Leftrightarrow \quad \boldsymbol{F}_k \boldsymbol{u} = \boldsymbol{0}, \tag{3.3}$$

where we have defined

$$\boldsymbol{F}_p = [\,\boldsymbol{f}_0 \,|\, \boldsymbol{f}_1 \,|\, \cdots \,|\boldsymbol{f}_p\,] \in \mathbb{C}^{N\times(p+1)}, \quad \boldsymbol{u} = [u_0, u_1, \ldots, u_k]^T. \tag{3.4}$$

In order for this approach to be valid, we need to show that the system of N equations in (3.3) has a unique solution normalized such that $u_k = 1$. With this normalization, (3.3) becomes

$$\sum_{j=0}^{k-1} u_j \boldsymbol{f}_j = -\boldsymbol{f}_k \quad \Leftrightarrow \quad \boldsymbol{F}_{k-1}\boldsymbol{u}' = -\boldsymbol{f}_k, \quad \boldsymbol{u}' = [u_0, u_1, \ldots, u_{k-1}]^T. \tag{3.5}$$

Define the matrices $\boldsymbol{A} \in \mathbb{C}^{N\times k}$ and $\boldsymbol{V} \in \mathbb{C}^{k\times k}$ as in

$$\boldsymbol{A} = [\,\boldsymbol{a}_1\,|\,\boldsymbol{a}_2\,|\,\cdots\,|\,\boldsymbol{a}_k\,], \quad \boldsymbol{V} = \begin{bmatrix} 1 & \zeta_1 & \cdots & \zeta_1^{k-1} \\ 1 & \zeta_2 & \cdots & \zeta_2^{k-1} \\ \vdots & \vdots & & \vdots \\ 1 & \zeta_k & \cdots & \zeta_k^{k-1} \end{bmatrix}. \tag{3.6}$$

Then the matrix $\boldsymbol{F}_{k-1}$ in (3.5) is of the form

$$\boldsymbol{F}_{k-1} = \boldsymbol{AV}. \tag{3.7}$$

Since the matrix $\boldsymbol{V}$ is nonsingular because the ζ_i are distinct, we have $\operatorname{rank}(\boldsymbol{F}_{k-1}) = \operatorname{rank}(\boldsymbol{A}) = k$. Therefore, (3.5) has a unique solution for $\boldsymbol{u}'$.

The solution of (3.3) can be achieved in one of the following ways:

1. *Solution via linear least-squares:* Setting $u_k = 1$ in (3.3), we can use standard least squares to solve (3.5) for $\boldsymbol{u}'$. Thus,

$$\min_{\boldsymbol{u}'} \|\boldsymbol{F}_{k-1}\boldsymbol{u}' + \boldsymbol{f}_k\| \quad \Rightarrow \quad \boldsymbol{u}' = -\boldsymbol{F}_{k-1}^{+}\boldsymbol{f}_k. \tag{3.8}$$

Here $\boldsymbol{K}^+$ denotes the Moore–Penrose generalized inverse of the matrix $\boldsymbol{K}$. This amounts to forcing the vector $\sum_{j=0}^{k} u_j \boldsymbol{f}_j$ to be orthogonal to the subspace $\operatorname{span}\{\boldsymbol{f}_0, \boldsymbol{f}_1, \ldots, \boldsymbol{f}_{k-1}\}$.

Since $\boldsymbol{F}_{k-1}$ has full column rank, we can solve (3.8) via QR factorization of $\boldsymbol{F}_k$, namely, via

$$\boldsymbol{F}_k = \boldsymbol{Q}_k\boldsymbol{R}_k, \quad \boldsymbol{Q}_k \text{ unitary}, \quad \boldsymbol{R}_k \text{ upper triangular}, \tag{3.9}$$

$$\boldsymbol{Q}_k = [\,\boldsymbol{q}_0\,|\,\boldsymbol{q}_1\,|\,\cdots\,|\,\boldsymbol{q}_k\,] \in \mathbb{C}^{N\times(k+1)}, \quad \boldsymbol{q}_i^*\boldsymbol{q}_j = \delta_{ij}, \tag{3.10}$$

and

$$\boldsymbol{R}_k = \begin{bmatrix} r_{00} & r_{01} & \cdots & r_{0k} \\ & r_{11} & \cdots & r_{1k} \\ & & \ddots & \vdots \\ & & & r_{kk} \end{bmatrix}, \quad r_{ii} > 0 \ \ \forall\, i \le k. \tag{3.11}$$

Noting that

$$\boldsymbol{Q}_k = [\,\boldsymbol{Q}_{k-1}\,|\,\boldsymbol{q}_k\,]; \quad \boldsymbol{R}_k = \left[\begin{array}{c|c} \boldsymbol{R}_{k-1} & \boldsymbol{\rho}_k \\ \hline \boldsymbol{0}^{\mathrm{T}} & r_{kk} \end{array}\right], \quad \boldsymbol{\rho}_k = [r_{0k}, r_{1k}, \ldots, r_{k-1,k}]^T \in \mathbb{C}^k, \tag{3.12}$$

we have that $\boldsymbol{u}'$ ultimately satisfies the $k \times k$ nonsingular upper triangular linear system

$$\boldsymbol{R}_{k-1}\boldsymbol{u}' = -\boldsymbol{\rho}_k, \tag{3.13}$$

which can be solved by back substitution.

This method turns out to be a special case of that derived from the vector-valued rational approximation procedure called *SMPE*, which we describe in the next section. The algorithm that uses the QR factorization described above also resembles an analogous algorithm used in [13] for the scalar Prony problem.

2. *Solution via singular value decomposition:* Note that the least-squares problem in (3.8) is *unconstrained*. We can also obtain the u_j (with a different normalization) as the solution to the following *constrained* least-squares problem:

$$\min_{\boldsymbol{u}} \|\boldsymbol{F}_k\boldsymbol{u}\| \quad \text{subject to} \quad \|\boldsymbol{u}\| = 1. \tag{3.14}$$

The solution for $\boldsymbol{u}$ is now the right singular vector of $\boldsymbol{F}_k$ corresponding to its smallest singular value (which is now zero, since the system $\boldsymbol{F}_k\boldsymbol{u} = \boldsymbol{0}$ is consistent). Of course, this can be achieved via the singular value decomposition (SVD) of $\boldsymbol{F}_k$. The u_j are now normalized via $\sum_{j=0}^{k}|u_j|^2 = 1$.

Now, as suggested by Chan [3], the SVD of the $N \times (k+1)$ matrix $\boldsymbol{F}_k$ can be obtained in a convenient way from the SVD of the $(k+1) \times (k+1)$ matrix $\boldsymbol{R}_k$ that results from the QR factorization of $\boldsymbol{F}_k$ in (3.9)–(3.11).[1]

Let $\boldsymbol{R}_k = \boldsymbol{W}\boldsymbol{\Sigma}\boldsymbol{V}^*$ be the SVD of $\boldsymbol{R}_k$, where all three matrices $\boldsymbol{W}$, $\boldsymbol{V}$, and $\boldsymbol{\Sigma}$ are square, $\boldsymbol{W}$ and $\boldsymbol{V}$ are unitary, and $\boldsymbol{\Sigma} = \text{diag}(\sigma_0, \sigma_1, \ldots, \sigma_k)$, $\sigma_0 \geq \sigma_1 \geq \cdots \geq \sigma_k$ being the singular values of $\boldsymbol{R}_k$. Then $\boldsymbol{F}_k = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^*$ is the SVD of $\boldsymbol{F}_k$ because $\boldsymbol{U} = \boldsymbol{Q}_k\boldsymbol{W}$ is unitary. In fact, the singular values and the corresponding right singular vectors of $\boldsymbol{F}_k$ are precisely those of $\boldsymbol{R}_k$. Thus, if $\boldsymbol{V} = [\,\boldsymbol{v}_0\,|\,\boldsymbol{v}_1\,|\,\cdots\,|\,\boldsymbol{v}_k\,]$, then, for $i = 0, 1, \ldots, k$, $\boldsymbol{v}_i$ is the right singular vector of $\boldsymbol{F}_k$ corresponding to the singular value σ_i.

Therefore, by the way the σ_i are ordered in the matrix $\boldsymbol{\Sigma}$, σ_k is the smallest singular value of $\boldsymbol{F}_k$ and, therefore, the solution to (3.14) is $\boldsymbol{u} = \boldsymbol{v}_k$. In addition, $\sigma_k = 0$ because the linear system $\boldsymbol{F}_k\boldsymbol{u} = \boldsymbol{0}$ is consistent in our case. [Of course, when errors are present in the $\boldsymbol{f}_m$, then $\sigma_k > 0$ will hold in general. Nevertheless, we can take the vector $\boldsymbol{v}_k$ as our (approximate) solution for $\boldsymbol{u}$.]

3. *Solution via Gaussian elimination with partial pivoting:* Setting $u_k = 1$ in (3.3), we have the $N \times k$ system (3.5). Choosing k linearly independent vectors $\boldsymbol{g}_1, \ldots, \boldsymbol{g}_k$ in $\mathbb{C}^N$, and taking the inner product of these vectors with (3.5), we obtain the $k \times k$ linear system

$$\sum_{j=0}^{k-1}(\boldsymbol{g}_i, \boldsymbol{f}_j)u_j = -(\boldsymbol{g}_i, \boldsymbol{f}_k), \quad i = 1, \ldots, k. \tag{3.15}$$

Letting

$$\boldsymbol{G} = [\,\boldsymbol{g}_1\,|\,\boldsymbol{g}_2\,|\,\cdots\,|\,\boldsymbol{g}_k\,] \in \mathbb{C}^{N\times k},$$

we can express this system in matrix form as follows:

$$\boldsymbol{G}^*\boldsymbol{F}_{k-1}\boldsymbol{u}' = -\boldsymbol{G}^*\boldsymbol{f}_k. \tag{3.16}$$

Of course, we should also make sure that the matrix $\boldsymbol{G}$ is such that $\boldsymbol{G}^*\boldsymbol{F}_{k-1} \in \mathbb{C}^{k\times k}$ is nonsingular; that $\text{rank}(\boldsymbol{G}) = \text{rank}(\boldsymbol{F}_{k-1}) = k$ is not sufficient. Taking

[1] Note that $\boldsymbol{R}_k$ is a much smaller matrix to handle than $\boldsymbol{F}_k$ in case $N >> k$.

the $\boldsymbol{g}_i$ to be k standard basis vectors amounts to picking k of the N scalar equations from (3.5). A good strategy amounting precisely to this approach is to use Gaussian elimination with partial pivoting on the matrix $\boldsymbol{F}_k$. Thus, there exists a permutation matrix $\boldsymbol{P} \in \mathbb{C}^{N\times N}$ depending on k, implying $\boldsymbol{G}^* = \boldsymbol{P}$ in (3.16), such that

$$\boldsymbol{P}\boldsymbol{F}_{k-1}\boldsymbol{u}' = -\boldsymbol{P}\boldsymbol{f}_k, \quad \boldsymbol{P}\boldsymbol{F}_k = \boldsymbol{L}_k\boldsymbol{U}_k, \tag{3.17}$$

where $\boldsymbol{L}_k$ is a lower trapezoidal matrix and $\boldsymbol{U}_k$ is an upper triangular matrix. We have

$$\boldsymbol{L}_k = \left[\frac{\boldsymbol{L}_k'}{\boldsymbol{L}_k''}\right], \quad \boldsymbol{L}_k' \in \mathbb{C}^{(k+1)\times(k+1)}, \quad \boldsymbol{L}_k'' \in \mathbb{C}^{(N-k-1)\times(k+1)},$$

$\boldsymbol{L}_k'$ being lower triangular with ones along its diagonal. (As a result of partial pivoting, all entries of $\boldsymbol{L}_k$ below the diagonal are at most unity in modulus.) In addition, $\boldsymbol{L}_k$ and $\boldsymbol{U}_k$ can be partitioned as in

$$\boldsymbol{L}_k = \left[\begin{array}{c|c} \boldsymbol{L}_{k-1}' & \boldsymbol{0} \\ \hline \boldsymbol{L}_{k-1}'' & \boldsymbol{l}_k \end{array}\right], \quad \boldsymbol{l}_k \in \mathbb{C}^{N-k}; \quad \boldsymbol{U}_k = \left[\begin{array}{c|c} \boldsymbol{U}_{k-1} & \boldsymbol{\sigma}_k \\ \hline \boldsymbol{0}^{\mathrm{T}} & \sigma_{kk} \end{array}\right], \quad \boldsymbol{\sigma}_k \in \mathbb{C}^k, \tag{3.18}$$

$\boldsymbol{U}_{k-1}$ being nonsingular. With these developments, the first k of the N equations in (3.17) give the $k \times k$ nonsingular upper triangular linear system

$$\boldsymbol{U}_{k-1}\boldsymbol{u}' = -\boldsymbol{\sigma}_k, \tag{3.19}$$

which can be solved for $\boldsymbol{u}'$ by back substitution.

This method turns out to be a special case of that derived from the vector-valued rational approximation procedure called *SMMPE*, which we describe in the next section.

3.2.2 The case $a_1, \ldots, a_k$ are linearly dependent

When the vectors $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_k$ are linearly dependent, the methods proposed above cannot be applied. This situation happens naturally when $k > N$. It may happen even when $k \le N$.[2] The method we propose next is applicable in these cases; actually, it can be applied always, whether $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_k$ are linearly dependent or not.

Choose an arbitrary vector $\boldsymbol{g}$ and take its inner product with the equations in (3.2), and consider those equations with $m = 0, 1, \ldots, k-1$. This gives the $k \times k$ linear system

$$\sum_{j=0}^{k-1} (\boldsymbol{g}, \boldsymbol{f}_{m+j})u_j = -(\boldsymbol{g}, \boldsymbol{f}_{m+k}), \quad m = 0, 1, \ldots, k-1, \tag{3.20}$$

[2] Such vector sequences can always be generated by a linear recursion of the form

$$\sum_{j=0}^{m} \boldsymbol{A}_j \boldsymbol{f}_{k+j} = \boldsymbol{0}, \quad k = 0, 1, \ldots,$$

where $\boldsymbol{A}_j \in \mathbb{C}^{N\times N}$, $j = 0, 1, \ldots, m$, $\boldsymbol{A}_m$ is nonsingular, and $\boldsymbol{A}_0 \ne \boldsymbol{O}$. For details, see the note by Sidi [24], for example.

for $u_0, u_1, \ldots, u_{k-1}$, with $u_k = 1$ as before. This amounts to equating the projections along $\boldsymbol{g}$ of the k vectors $\sum_{j=0}^{k} u_j \boldsymbol{f}_{m+j}$, $m = 0, 1, \ldots, k-1$, to zero. [As we will see shortly, the vector $\boldsymbol{g}$ must be such that (3.24) must be satisfied.] To show that a unique solution for the u_j is provided by this system, we need to show that the matrix of this system, namely, the matrix

$$\widehat{\boldsymbol{T}}_{k-1} = \begin{bmatrix} (\boldsymbol{g}, \boldsymbol{f}_0) & (\boldsymbol{g}, \boldsymbol{f}_1) & \cdots & (\boldsymbol{g}, \boldsymbol{f}_{k-1}) \\ (\boldsymbol{g}, \boldsymbol{f}_1) & (\boldsymbol{g}, \boldsymbol{f}_2) & \cdots & (\boldsymbol{g}, \boldsymbol{f}_k) \\ \vdots & \vdots & & \vdots \\ (\boldsymbol{g}, \boldsymbol{f}_{k-1}) & (\boldsymbol{g}, \boldsymbol{f}_k) & \cdots & (\boldsymbol{g}, \boldsymbol{f}_{2k-2}) \end{bmatrix}, \tag{3.21}$$

is nonsingular. Now, it can easily be verified that

$$\widehat{\boldsymbol{T}}_{k-1} = \boldsymbol{V} \operatorname{diag}[(\boldsymbol{g}, \boldsymbol{a}_1), \ldots, (\boldsymbol{g}, \boldsymbol{a}_k)]\, \boldsymbol{V}^T, \tag{3.22}$$

where $\boldsymbol{V}$ is the Vandermonde matrix defined in (3.6). Since all three matrices here are $k \times k$, we have that

$$\det \widehat{\boldsymbol{T}}_{k-1} = \left[\prod_{i=1}^{k} (\boldsymbol{g}, \boldsymbol{a}_i) \right] (\det \boldsymbol{V})^2, \tag{3.23}$$

which is nonzero if and only if

$$\prod_{i=1}^{k} (\boldsymbol{g}, \boldsymbol{a}_i) \neq 0. \tag{3.24}$$

Thus, $\widehat{\boldsymbol{T}}_{k-1}$ is nonsingular provided (3.24) is satisfied.

This method turns out to be a special case of that derived from the vector-valued rational approximation procedure called *STEA*, which we describe in the next section.

3.3 Determination of $a_1, \ldots, a_k$

With the u_j and hence the ζ_i determined, we turn to the problem of determining the $\boldsymbol{a}_i$. We do this basically as explained in Section 2, by resorting to the Padé approximant approach.

It is clear that the vector-valued rational function

$$\boldsymbol{f}_{k-1,k}(z) = \frac{\sum_{j=0}^{k} u_j z^{k-j} \boldsymbol{s}_{j-1}(z)}{\sum_{j=0}^{k} u_j z^{k-j}}, \tag{3.25}$$

where

$$\boldsymbol{s}_m(z) = \sum_{j=0}^{m} \boldsymbol{f}_j z^j, \quad m = 0, 1, \ldots; \quad \boldsymbol{s}_m(z) \equiv \boldsymbol{0} \ \text{ if } m < 0, \tag{3.26}$$

is the $[k-1/k]$ Padé approximant to $\boldsymbol{f}(z) = \sum_{j=0}^{\infty} \boldsymbol{f}_j z^j$ componentwise, and has the partial fraction decomposition

$$\boldsymbol{f}_{k-1,k}(z) = \sum_{i=1}^{k} \frac{\boldsymbol{w}_i}{z - z_i}. \tag{3.27}$$

In addition, by (2.8), we also have

$$\boldsymbol{f}(z) = \sum_{i=1}^{k} \frac{\boldsymbol{a}_i}{1 - \zeta_i z}, \tag{3.28}$$

and, therefore,

$$\boldsymbol{f}_{k-1,k}(z) \equiv \boldsymbol{f}(z). \tag{3.29}$$

Consequently,

$$\zeta_i = z_i^{-1}, \quad \boldsymbol{a}_i = -\boldsymbol{w}_i z_i^{-1}, \quad i = 1, \ldots, k, \tag{3.30}$$

the $\boldsymbol{w}_i$ being computed as in

$$\boldsymbol{w}_i = \operatorname{Res} \boldsymbol{f}_{k-1,k}(z)\Big|_{z=z_i} = \frac{\sum_{j=0}^{k} u_j z^{k-j} \boldsymbol{s}_{j-1}(z)}{\sum_{j=0}^{k} (k-j) u_j z^{k-j-1}}\Bigg|_{z=z_i}, \quad i = 1, \ldots, k. \tag{3.31}$$

Remark When everything—the determination of the ζ_i and the $\boldsymbol{a}_i$—is taken into account, it is seen that the necessary input for the algorithms described above is

- the $k+1$ vectors $\boldsymbol{f}_0, \boldsymbol{f}_1, \ldots, \boldsymbol{f}_k$ in case $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_k$ are linearly independent,
- the $2k$ vectors $\boldsymbol{f}_0, \boldsymbol{f}_1, \ldots, \boldsymbol{f}_{2k-1}$ in case $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_k$ are linearly dependent.

4 Prony-like algorithms for vector problems via vector-valued rational approximations

4.1 A reduced Prony problem

In this section, we again consider vector sequences $\{\boldsymbol{f}_m\}_{m=0}^{\infty}$ that satisfy

$$\boldsymbol{f}_m = \sum_{i=1}^{r} \boldsymbol{a}_i \zeta_i^m, \quad m = 0, 1, \ldots, \tag{4.1}$$

where $\boldsymbol{a}_i \in \mathbb{C}^N$ and $\zeta_i \in \mathbb{C}$ are independent of m, ζ_i are distinct, and r may be very large, even infinite. Of course, when $r = \infty$, the methods we discussed in the previous section cannot be applied for determining *all* of the ζ_i and $\boldsymbol{a}_i$. Similarly, when r is finite but very large, the application of the methods we discussed in the previous section for determining *all* of the ζ_i and $\boldsymbol{a}_i$ becomes very expensive. In view of this limitation, we change/reduce the classical Prony problem as follows:

Approximate the k largest (in modulus) ζ_i and the corresponding $\boldsymbol{a}_i$, instead of all r of the pairs $(\zeta_i, \boldsymbol{a}_i)$. Ordering the ζ_i such that

$$|\zeta_1| \geq |\zeta_2| \geq \cdots \geq |\zeta_r|, \tag{4.2}$$

we would like to approximate the pairs $(\zeta_i, \boldsymbol{a}_i)$, $i = 1, \ldots, k$, with $k < r$. Of course, this amounts to approximating $\boldsymbol{f}_m$ in (4.1) by the sum $\sum_{i=1}^{k} \boldsymbol{a}_i \zeta_i^m$.

We can achieve our goal by using some vector-valued rational approximation procedures when the ζ_i are such that $|\zeta_k| > |\zeta_{k+1}|$.[3] In particular, we can use SMPE, SMMPE, and STEA, three procedures that were developed and analyzed in Sidi [20]. The connection of these procedures with Krylov subspace methods was shown in Sidi [21]. SMPE has been applied by Wu, Li, and Li [27] to problems in reanalysis of structures and by Wu and Zhong [28] to nonlinear differential equations with a small parameter. For an extensive summary, see also Sidi [23, Chapters 12, 14]. We introduce the essentials of this subject that are relevant to our aim next.

4.2 Vector-valued rational approximations

We start by recalling that the series $\sum_{j=0}^{\infty} \boldsymbol{f}_j z^j$ represents the (rational) function

$$\boldsymbol{f}(z) = \sum_{i=1}^{r} \frac{\boldsymbol{a}_i}{1 - \zeta_i z}, \tag{4.3}$$

which can also be expressed as

$$\boldsymbol{f}(z) = \sum_{i=1}^{r} \frac{\boldsymbol{w}_i}{z - z_i}; \quad z_i = \zeta_i^{-1}, \quad \boldsymbol{w}_i = -\boldsymbol{a}_i \zeta_i^{-1}, \quad i = 1, \ldots, r. \tag{4.4}$$

Therefore, (4.2) implies

$$|z_1| \leq |z_2| \cdots \leq |z_r|. \tag{4.5}$$

[Clearly, the numerator of $\boldsymbol{f}(z)$ is a vector-valued polynomial of degree at most $r-1$, while its denominator is a scalar polynomial of degree r.] We apply the three rational approximation procedures mentioned above to the sequence of the partial sums

$$\boldsymbol{s}_m(z) = \sum_{j=0}^{m} \boldsymbol{f}_j z^j, \quad m = 0, 1, \ldots. \tag{4.6}$$

All three procedures produce vector-valued rational functions $\boldsymbol{s}_{n,k}(z)$ that approximate $\boldsymbol{f}(z)$ and that can be expressed in the form

$$\boldsymbol{s}_{n,k}(z) = \frac{\boldsymbol{p}_{n,k}(z)}{q_{n,k}(z)} = \frac{\sum_{j=0}^{k} u_j z^{k-j} \boldsymbol{s}_{n+j}(z)}{\sum_{j=0}^{k} u_j z^{k-j}}, \quad q_{n,k}(0) = u_k = 1, \tag{4.7}$$

[3] A case of interest can be as follows: The first k of the ζ_i, namely, $\zeta_1, \ldots, \zeta_k$, are on the unit disk, while the rest are in the interior of the unit disk. Thus, $\boldsymbol{f}_m = \boldsymbol{f}_m^{(1)} + \boldsymbol{f}_m^{(2)}$, with $\boldsymbol{f}_m^{(1)} = \sum_{i=1}^{k} \boldsymbol{a}_i \zeta_i^m$ and $\boldsymbol{f}_m^{(2)} = \sum_{i=k+1}^{r} \boldsymbol{a}_i \zeta_i^m$. Of these, $\boldsymbol{f}_m^{(1)}$ is what we need to obtain/approximate, while $\boldsymbol{f}_m^{(2)}$ is a *transient*, that is, $\lim_{m\to\infty} \boldsymbol{f}_m^{(2)} = \boldsymbol{0}$.

where the u_j are scalars to be determined. It is clear that $\boldsymbol{p}_{n,k}(z)$ is a vector-valued polynomial of degree at most $n+k$, while $q_{n,k}(z)$ is a scalar polynomial of degree k. In addition, for *any* set of $u_0, u_1, \ldots, u_{k-1}$,

$$\boldsymbol{f}(z) - \boldsymbol{s}_{n,k}(z) = \frac{\sum_{j=0}^{k} u_j z^{k-j}[\boldsymbol{f}(z) - \boldsymbol{s}_{n+j}(z)]}{\sum_{j=0}^{k} u_j z^{k-j}} = O(z^{n+k+1}) \quad \text{as } z \to 0; \tag{4.8}$$

that is, $\boldsymbol{s}_{n,k}(z)$ interpolates $\boldsymbol{f}(z)$ at $z = 0$ in the sense of Hermite $n+k+1$ times, thus has a Padé-like behavior; it is *not* a Padé approximant, however.[4]

Letting

$$\boldsymbol{F}_{n,p} = [\,\boldsymbol{f}_n \,|\, \boldsymbol{f}_{n+1} \,|\, \cdots \,|\, \boldsymbol{f}_{n+p}\,] \tag{4.9}$$

and

$$\widehat{\boldsymbol{T}}_{n,p} = \begin{bmatrix} (\boldsymbol{g}, \boldsymbol{f}_n) & (\boldsymbol{g}, \boldsymbol{f}_{n+1}) & \cdots & (\boldsymbol{g}, \boldsymbol{f}_{n+p}) \\ (\boldsymbol{g}, \boldsymbol{f}_{n+1}) & (\boldsymbol{g}, \boldsymbol{f}_{n+2}) & \cdots & (\boldsymbol{g}, \boldsymbol{f}_{n+p+1}) \\ \vdots & \vdots & & \vdots \\ (\boldsymbol{g}, \boldsymbol{f}_{n+p}) & (\boldsymbol{g}, \boldsymbol{f}_{n+p+1}) & \cdots & (\boldsymbol{g}, \boldsymbol{f}_{n+2p}) \end{bmatrix}, \tag{4.10}$$

we turn to the issue of determining $u_0, u_1, \ldots, u_{k-1}$ with the normalization $u_k = 1$.

- *For SMPE:* Solve by least squares

$$\sum_{j=0}^{k-1} \boldsymbol{f}_{n+j} u_j = -\boldsymbol{f}_{n+k} \quad \Leftrightarrow \quad \boldsymbol{F}_{n,k-1}\boldsymbol{u}' = -\boldsymbol{f}_{n+k}. \tag{4.11}$$

This amounts to solving the minimization problem

$$\min_{\boldsymbol{u}'} \|\boldsymbol{F}_{n,k-1}\boldsymbol{u}' + \boldsymbol{f}_{n+k}\| \quad \Rightarrow \quad \boldsymbol{u}' = -\boldsymbol{F}^{+}_{n,k-1}\boldsymbol{f}_{n+k}, \tag{4.12}$$

which amounts to forcing the vector $\sum_{j=0}^{k-1} u_j \boldsymbol{f}_{n+j} + \boldsymbol{f}_{n+k}$ to be orthogonal to the subspace $\text{span}\{\boldsymbol{f}_n, \boldsymbol{f}_{n+1}, \ldots, \boldsymbol{f}_{n+k-1}\}$, and results in the system of normal equations

$$\sum_{j=0}^{k-1} f_{i,j} u_j = -f_{i,k}, \quad i = 0, 1, \ldots, k-1; \quad f_{i,j} = (\boldsymbol{f}_{n+i}, \boldsymbol{f}_{n+j}). \tag{4.13}$$

The solution for $u_0, u_1, \ldots, u_{k-1}$ can be achieved precisely as described in (3.8)–(3.13), by replacing $\boldsymbol{F}_{k-1}$ there by $\boldsymbol{F}_{n,k-1}$. [Note that the equations in (4.11) are *not* consistent, hence do not have a solution in the regular sense.]

[4]Of course, in order for $\boldsymbol{s}_{n,k}(z)$ to be a reasonable approximation to $\boldsymbol{f}(z)$, the u_j should depend on $\boldsymbol{f}(z)$. Thus, in case only the $\boldsymbol{f}_j$ are known, the u_j should depend on the $\boldsymbol{f}_j$. This is indeed the case for SMPE, SMMPE, and STEA.

- *For SMMPE:* Choose k linearly independent vectors $\boldsymbol{g}_1, \ldots, \boldsymbol{g}_k$ and demand that the projection of the vector $\sum_{j=0}^{k-1} \boldsymbol{f}_{n+j} u_j + \boldsymbol{f}_{n+k}$ onto the subspace span$\{\boldsymbol{g}_1, \ldots, \boldsymbol{g}_k\}$ vanish. This results in the system of equations

$$\sum_{j=0}^{k-1} f_{i,j} u_j = -f_{i,k}, \quad i = 0, 1, \ldots, k-1; \quad f_{i,j} = (\boldsymbol{g}_{i+1}, \boldsymbol{f}_{n+j}). \tag{4.14}$$

  The solution for $u_0, u_1, \ldots, u_{k-1}$ can be achieved precisely as described in (3.17)–(3.19), by replacing $\boldsymbol{F}_{k-1}$ there by $\boldsymbol{F}_{n,k-1}$.
- *For STEA:* Choose a vector $\boldsymbol{g}$ and demand that the projections of the k vectors $\sum_{j=0}^{k-1} \boldsymbol{f}_{m+j} u_j + \boldsymbol{f}_{m+k}$, $m = n, n+1, \ldots, n+k-1$, along $\boldsymbol{g}$ vanish. This results in the system of equations

$$\sum_{j=0}^{k-1} f_{i,j} u_j = -f_{i,k}, \quad i = 0, 1, \ldots, k-1; \quad f_{i,j} = (\boldsymbol{g}, \boldsymbol{f}_{n+i+j}). \tag{4.15}$$

  The solution for $u_0, u_1, \ldots, u_{k-1}$ can be achieved precisely as described in (3.20)–(3.21), by replacing the matrix $\widehat{\boldsymbol{T}}_{k-1}$ there by $\widehat{\boldsymbol{T}}_{n,k-1}$.

Once $u_0, u_1, \ldots, u_{k-1}$ have been determined, the zeros $\zeta_i^{(n,k)}$, $i = 1, \ldots, k$, of the polynomial $u(\zeta) = \sum_{j=0}^{k} u_j \zeta^j$ (with $u_k = 1$) are the required approximations to ζ_i, $i = 1, \ldots, k$.[5]

The linear equations in (4.13)–(4.15) that produce the u_j in (4.7) also result in the (unified) determinant representation for $\boldsymbol{s}_{n,k}(z)$ from SMPE, SMMPE, and STEA, given as

$$\boldsymbol{s}_{n,k}(z) = \frac{\begin{vmatrix} z^k \boldsymbol{s}_n(z) & z^{k-1} \boldsymbol{s}_{n+1}(z) & \cdots & z^0 \boldsymbol{s}_{n+k}(z) \\ f_{0,0} & f_{0,1} & \cdots & f_{0,k} \\ f_{1,0} & f_{1,1} & \cdots & f_{1,k} \\ \vdots & \vdots & & \vdots \\ f_{k-1,0} & f_{k-1,1} & \cdots & f_{k-1,k} \end{vmatrix}}{\begin{vmatrix} z^k & z^{k-1} & \cdots & z^0 \\ f_{0,0} & f_{0,1} & \cdots & f_{0,k} \\ f_{1,0} & f_{1,1} & \cdots & f_{1,k} \\ \vdots & \vdots & & \vdots \\ f_{k-1,0} & f_{k-1,1} & \cdots & f_{k-1,k} \end{vmatrix}} \equiv \frac{\hat{\boldsymbol{p}}_{n,k}(z)}{\hat{q}_{n,k}(z)}, \tag{4.16}$$

with

$$f_{i,j} = \begin{cases} (\boldsymbol{f}_{n+i}, \boldsymbol{f}_{n+j}) & \text{for SMPE,} \\ (\boldsymbol{g}_{i+1}, \boldsymbol{f}_{n+j}) & \text{for SMMPE,} \\ (\boldsymbol{g}, \boldsymbol{f}_{n+i+j}) & \text{for STEA.} \end{cases} \tag{4.17}$$

[5] In Section 4.4, we show that the ζ_i for each of the three methods can also be obtained by solving an associated generalized eigenvalue problem, without having to solve the polynomial equation $u(\zeta) = \sum_{j=0}^{k} u_j \zeta^j = 0$.

4.3 Montessus- and König-type convergence theory

The following theorem from [20] concerns the convergence properties of all three interpolation procedures as $n \to \infty$ with k fixed. We also note that an interesting phenomenon takes place concerning the ζ_i when the vectors $\boldsymbol{a}_i$ are mutually orthogonal; see (4.21)–(4.22) and also Remark 1 following the statement of the theorem.

Theorem 4.1 *Let $\{\boldsymbol{f}_m\}$ and $\boldsymbol{f}(z)$ be as in (4.1)–(4.5), and that, for some $k < r$,*

$$|\zeta_k| > |\zeta_{k+1}| \quad \Leftrightarrow \quad |z_k| < |z_{k+1}|.$$

Assume also that

$$\boldsymbol{a}_1, \ldots, \boldsymbol{a}_k \ \text{ are linearly independent for SMPE and SMMPE,}$$

$$\begin{vmatrix} (\boldsymbol{g}_1, \boldsymbol{a}_1) & (\boldsymbol{g}_1, \boldsymbol{a}_2) & \cdots & (\boldsymbol{g}_1, \boldsymbol{a}_k) \\ (\boldsymbol{g}_2, \boldsymbol{a}_1) & (\boldsymbol{g}_2, \boldsymbol{a}_2) & \cdots & (\boldsymbol{g}_2, \boldsymbol{a}_k) \\ \vdots & \vdots & & \vdots \\ (\boldsymbol{g}_k, \boldsymbol{a}_1) & (\boldsymbol{g}_k, \boldsymbol{a}_2) & \cdots & (\boldsymbol{g}_k, \boldsymbol{a}_k) \end{vmatrix} \neq 0 \quad \text{for SMMPE,}$$

$$(\boldsymbol{g}, \boldsymbol{a}_i) \neq 0, \quad i = 1, \ldots, k, \quad \text{for STEA.}$$

Then the following are true:

1. *Define $K_k = \{z : |z| < |z_{k+1}|\}$. Then $\boldsymbol{s}_{n,k}(z)$ exists for all sufficiently large n. It converges to $\boldsymbol{f}(z)$ as $n \to \infty$ uniformly in z, in every compact subset of $K_k \setminus \{z_1, \ldots, z_k\}$, such that*

$$\boldsymbol{s}_{n,k}(z) = \boldsymbol{f}(z) + O(|z/z_{k+1}|^n) \quad \text{as } n \to \infty. \tag{4.18}$$

2. *The polynomial $q_{n,k}(z)$ exists for all sufficiently large n and*

$$\lim_{n\to\infty} q_{n,k}(z) = \prod_{i=1}^{k}(1 - \zeta_i z)$$

as in

$$q_{n,k}(z) = \prod_{i=1}^{k}(1 - \zeta_i z) + O(|\zeta_{k+1}/\zeta_k|^n) \quad \text{as } n \to \infty. \tag{4.19}$$

$q_{n,k}(z)$ has k zeros $z_1^{(n,k)}, \ldots, z_k^{(n,k)}$, that converge to the poles $z_1, \ldots, z_k$, as in

$$z_i^{(n,k)} - z_i = O(|\zeta_{k+1}/\zeta_i|^n) \quad \text{as } n \to \infty, \quad i = 1, \ldots, k. \tag{4.20}$$

In case the vectors $\boldsymbol{a}_i$ are mutually orthogonal, that is, $(\boldsymbol{a}_i, \boldsymbol{a}_j) = 0$ if $i \neq j$, these results for SMPE improve to read

$$q_{n,k}(z) = \prod_{i=1}^{k}(1 - \zeta_i z) + O(|\zeta_{k+1}/\zeta_k|^{2n}) \quad \text{as } n \to \infty \tag{4.21}$$

and

$$z_i^{(n,k)} - z_i = O(|\zeta_{k+1}/\zeta_i|^{2n}) \quad \text{as } n \to \infty, \quad i = 1, \ldots, k. \tag{4.22}$$

3. *The residues of* $\boldsymbol{s}_{n,k}(z)$ *at its poles* $z_i^{(n,k)}$*, namely,* $\boldsymbol{w}_i^{(n,k)} = \operatorname{Res} \boldsymbol{s}_{n,k}(z)\big|_{z=z_i^{(n,k)}}$*, converge to the residues of* $\boldsymbol{f}(z)$ *at its poles* z_i*, as in*

$$\boldsymbol{w}_i^{(n,k)} = -z_i \boldsymbol{a}_i + O(|\zeta_{k+1}/\zeta_i|^n) \ \textit{as } n \to \infty, \quad i = 1, \ldots, k. \tag{4.23}$$

Thus, there holds

$$\boldsymbol{a}_i = -\boldsymbol{w}_i^{(n,k)}/z_i^{(n,k)} + O(|\zeta_{k+1}/\zeta_i|^n) \ \textit{as } n \to \infty, \quad i = 1, \ldots, k. \tag{4.24}$$

4. *When* $k = r$*, we have*

$$z_i^{(n,r)} = z_i \quad \Rightarrow \quad \zeta_i^{(n,r)} = \zeta_i, \quad i = 1, \ldots, r.$$

We also have

$$\boldsymbol{w}_i^{(n,r)} = \boldsymbol{w}_i \quad \Rightarrow \quad \boldsymbol{w}_i^{(n,r)}/z_i^{(n,r)} = -\boldsymbol{a}_i, \quad i = 1, \ldots, r.$$

That is, the ζ_i *and* $\boldsymbol{a}_i$ *are reproduced exactly when* $k = r$*.*[6]

Remarks:

1. By the relations $\zeta_i = 1/z_i$ and $\zeta_i^{(n,k)} = 1/z_i^{(n,k)}$, the results in (4.20) and (4.22) concerning the convergence of the $z_i^{(n,k)}$ are, of course, the same as

$$\zeta_i^{(n,k)} - \zeta_i = O(|\zeta_{k+1}/\zeta_i|^n) \quad \text{as } n \to \infty, \quad i = 1, \ldots, k, \tag{4.25}$$

in general, and

$$\zeta_i^{(n,k)} - \zeta_i = O(|\zeta_{k+1}/\zeta_i|^{2n}) \quad \text{as } n \to \infty, \quad i = 1, \ldots, k, \tag{4.26}$$

respectively, in the case of SMPE when the $\boldsymbol{a}_i$ are mutually orthogonal. No change takes place in (4.23)–(4.24), however.

2. When $|\zeta_1| = \cdots = |\zeta_k|$, $\zeta_1^{(n,k)}, \ldots, \zeta_k^{(n,k)}$ converge to the respective ζ_i at the same rate, namely,

$$\zeta_i^{(n,k)} - \zeta_i = O(|\zeta_{k+1}/\zeta_1|^{cn}) \quad \text{as } n \to \infty; \quad c = \begin{cases} 2 & \text{if } (\boldsymbol{a}_i, \boldsymbol{a}_j) = 0 \ \text{ when } i \neq j, \\ 1 & \text{otherwise.} \end{cases}$$

As for the residues, we have

$$-\zeta_i^{(n,k)} \boldsymbol{w}_i^{(n,k)} = \boldsymbol{a}_i + O(|\zeta_{k+1}/\zeta_1|^n) \quad \text{as } n \to \infty. \tag{4.27}$$

(See the case described in footnote.[3])

3. To determine the u_j, we need only (i) $\boldsymbol{f}_m$, $n \le m \le n+k$, for SMPE and SMMPE, and (ii) $\boldsymbol{f}_m$, $n \le m \le n+2k-1$, for STEA. On the other hand, for $\boldsymbol{s}_{n,k}(z)$ in all three cases, we also need $\boldsymbol{f}_m$, $0 \le m \le n-1$. Therefore, we may be led to think that these extra $\boldsymbol{f}_m$ will also be needed for computing the residues of $\boldsymbol{f}_{n,k}(z)$. This is not the case, however, as we show next.

   Letting

$$\boldsymbol{s}_{n+j}(z) = \boldsymbol{s}_{n-1}(z) + z^n \boldsymbol{x}_{n,j}(z), \quad \boldsymbol{x}_{n,j}(z) = \sum_{i=n}^{n+j} \boldsymbol{f}_i z^{i-n},$$

[6] We are thus back precisely at the vector versions of Prony's algorithm developed in Section 3.

we can express $\boldsymbol{s}_{n,k}(z)$ in (4.7) as

$$\begin{aligned}\boldsymbol{s}_{n,k}(z) &= \boldsymbol{s}_{n-1}(z) + z^n \frac{\sum_{j=0}^{k} u_j z^{k-j} \boldsymbol{x}_{n,j}(z)}{q_{n,k}(z)}\\ &= \boldsymbol{s}_{n-1}(z) + z^n \frac{\sum_{p=0}^{k} h_{p,k}(z) \boldsymbol{f}_{n+p}}{q_{n,k}(z)}, \quad h_{p,k}(z) = \sum_{j=p}^{k} u_j z^{k-j+p}.\end{aligned}$$

As a result,

$$\operatorname{Res} \boldsymbol{s}_{n,k}(z)\big|_{z=z_i^{(n,k)}} = z^n \frac{\sum_{p=0}^{k} h_{p,k}(z) \boldsymbol{f}_{n+p}}{q'_{n,k}(z)}\bigg|_{z=z_i^{(n,k)}},$$

since the residue of $\boldsymbol{s}_{n-1}(z)$ at every z is zero. Thus, the residues of $\boldsymbol{f}_{n,k}(z)$ at the poles $z_i^{(n,k)}$ do not depend on $\boldsymbol{f}_0, \boldsymbol{f}_1, \ldots, \boldsymbol{f}_{n-1}$.

4. These results show that, by taking n sufficiently large and by fixing k, we can use $\{\boldsymbol{f}_m\}_{m=n}^{n+k}$ in case of SMPE and SMMPE and $\{\boldsymbol{f}_m\}_{m=n}^{n+2k-1}$ in case of STEA to approximate $(\zeta_i, \boldsymbol{a}_i)$ by $(\zeta_i^{(n,k)}, \boldsymbol{a}_i^{(n,k)})$, $i = 1, \ldots, k$. The rate of convergence (as n increases) is best for $(\zeta_1, \boldsymbol{a}_1)$, followed by $(\zeta_2, \boldsymbol{a}_2)$, and so on.
5. The approach we have presented in this section is valid when the $\boldsymbol{f}_m$ satisfy

$$\boldsymbol{f}_m = \sum_{i=1}^{r} \boldsymbol{a}_i \zeta_i^m + \boldsymbol{r}_m; \quad \boldsymbol{r}_m = O(\rho^m) \quad \text{as } m \to \infty,$$

where

$$|\zeta_1| \geq |\zeta_2| \geq \cdots \geq |\zeta_r| > \rho \quad \text{for some } \rho > 0.$$

The first three parts of Theorem 4.1 hold in this case, both (i) when $k < r$ and (ii) when $k = r$ with $|\zeta_{r+1}| \equiv \rho$. Part 4 does not hold.
6. The approach we have presented in this section is valid also when the $\boldsymbol{f}_m$ satisfy

$$\boldsymbol{f}_m \sim \sum_{i=1}^{\infty} \boldsymbol{a}_i \zeta_i^m \quad \text{as } m \to \infty,$$

where

$$|\zeta_1| \geq |\zeta_2| \geq \cdots, \quad \lim_{i \to \infty} \zeta_i = 0,$$

by which we mean

$$\left\| \boldsymbol{f}_m - \sum_{i=1}^{s-1} \boldsymbol{a}_i \zeta_i^m \right\| = O(|\zeta_s|^m) \quad \text{as } m \to \infty, \quad \forall\, s \geq 0.$$

Theorem 4.1 holds in its entirety in this case.
7. In all cases, the vectors $\boldsymbol{f}_m$ can be in an infinite dimensional inner product space (for SMPE) or a normed space (for SMMPE and STEA). In particular, $\boldsymbol{f}_m$ can be functions $f_m(x)$ that are members of the L_2 space of functions with inner product $(\boldsymbol{f}_i, \boldsymbol{f}_j) = \int_a^b w(x) \overline{f_i(x)} f_j(x)\, dx$, for example. See [20] for details.
8. All the above concerning STEA is applicable when $N = 1$, that is, when the $\boldsymbol{f}_m$ (and, of course, the $\boldsymbol{a}_i$) are scalars. In this case, we are back at Padé approximants hence Prony's algorithm when $k = r$ in Theorem 4.1. In addition, everything

that we have mentioned in the preceding remarks applies to this case without any changes.

9. In Section 3, one of the methods we suggested for determining the vector $\boldsymbol{u} = [u_0, u_1, \ldots, u_k]^T$ was based on the SVD of the matrix $\boldsymbol{F}_k$ via (3.14). For the reduced problem we have considered in this section, we now propose to determine $\boldsymbol{u}$ via the SVD of the matrix $\boldsymbol{F}_{n,k} = [\,\boldsymbol{f}_n \,|\, \boldsymbol{f}_{n+1} \,|\, \cdots \,|\, \boldsymbol{f}_{n+k}\,]$ as the solution to the constrained minimization problem

$$\min_{\boldsymbol{u}} \|\boldsymbol{F}_{n,k}\boldsymbol{u}\| \quad \text{subject to} \quad \|\boldsymbol{u}\| = 1$$

precisely as described in Section 3. With $\boldsymbol{u}$ obtained this way, (i) we compute the approximations $\zeta_i^{(n,k}$ as the roots of the polynomial $u(\zeta) = \sum_{j=0}^{k} u_j \zeta^j$, (ii) we form the rational approximation $\boldsymbol{s}_{n,k}(z)$ precisely as in (4.6)–(4.7), and (iii) we proceed to the approximation of the $\boldsymbol{a}_i$ via $\boldsymbol{a}_i \approx -\boldsymbol{w}_i^{(n,k)}/z_i^{(n,k)}$, where $\boldsymbol{w}_i^{(n,k)} = \operatorname{Res} \boldsymbol{s}_{n,k}(z)\big|_{z=z_i^{(n,k)}}$, with $z_i^{(n,k)} = 1/\zeta_i^{(n,k)}$.

4.4 A related generalized eigenvalue problem

We have seen that the poles of the rational functions $\boldsymbol{s}_{n,k}(z)$, that is, the zeros $z_i^{(n,k)} = 1/\zeta_i^{(n,k)}$ of the denominator polynomials $q_{n,k}(z)$ in (4.7), are the required approximations to $z_i = 1/\zeta_i$, $i = 1, \ldots, k$. Since $\hat{q}_{n,k}(z)$, the denominator determinant of $\boldsymbol{s}_{n,k}(z)$ in (4.16)–(4.17) is a constant multiple of $q_{n,k}(z)$, these $z_i^{(n,k)} = 1/\zeta_i^{(n,k)}$ are also the zeros of $\hat{q}_{n,k}(z)$. Making the substitution $z = 1/\zeta$ in these denominator determinants, we have that the $\zeta_i^{(n,k)}$ are the solution to $\zeta^k \hat{q}_{n,k}(1/\zeta) = \det \boldsymbol{M}(\zeta) = 0$, where

$$\boldsymbol{M}(\zeta) = \begin{bmatrix} \zeta^0 & \zeta^1 & \cdots & \zeta^k \\ f_{0,0} & f_{0,1} & \cdots & f_{0,k} \\ f_{1,0} & f_{1,1} & \cdots & f_{1,k} \\ \vdots & \vdots & & \vdots \\ f_{k-1,0} & f_{k-1,1} & \cdots & f_{k-1,k} \end{bmatrix}. \tag{4.28}$$

Let us now preform the following elementary column transformations on $\boldsymbol{M}(\zeta)$, which do not change the value of $\det \boldsymbol{M}(\zeta)$:

For $i = k, k-1, \ldots, 1$ **do**

Multiply column i by ζ and subtract from column $i+1$ and overwrite column $i+1$.

end do (i)

As a result of these column operations, which do not change the value of $\zeta^k \hat{q}_{n,k}(1/\zeta)$, we obtain $\zeta^k \hat{q}_{n,k}(1/\zeta) = \det \widehat{\boldsymbol{M}}(\zeta) = 0$, where

$$\widehat{\boldsymbol{M}}(\zeta) = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ f_{0,0} & f_{0,1} - \zeta f_{0,0} & f_{0,2} - \zeta f_{0,1} & \cdots & f_{0,k} - \zeta f_{0,k-1} \\ f_{1,0} & f_{1,1} - \zeta f_{1,0} & f_{1,2} - \zeta f_{1,1} & \cdots & f_{1,k} - \zeta f_{1,k-1} \\ \vdots & \vdots & \vdots & & \vdots \\ f_{k-1,0} & f_{k-1,1} - \zeta f_{k-1,0} & f_{k-1,2} - \zeta f_{k-1,1} & \cdots & f_{k-1,k} - \zeta f_{k-1,k-1} \end{bmatrix}. \tag{4.29}$$

By expanding $\det \widehat{\boldsymbol{M}}(\zeta)$ with respect to its first row, we finally obtain the following generalized eigenvalue problem satisfied by $\zeta_i^{(n,k)}$, $i = 1, \ldots, k$:

$$\det(\boldsymbol{M}_1 - \zeta \boldsymbol{M}_0) = 0, \tag{4.30}$$

where

$$\boldsymbol{M}_0 = \begin{bmatrix} f_{0,0} & f_{0,1} & \cdots & f_{0,k-1} \\ f_{1,0} & f_{1,1} & \cdots & f_{1,k-1} \\ \vdots & \vdots & & \vdots \\ f_{k-1,0} & f_{k-1,1} & \cdots & f_{k-1,k-1} \end{bmatrix} \tag{4.31}$$

and

$$\boldsymbol{M}_1 = \begin{bmatrix} f_{0,1} & f_{0,2} & \cdots & f_{0,k} \\ f_{1,1} & f_{1,2} & \cdots & f_{1,k} \\ \vdots & \vdots & & \vdots \\ f_{k-1,1} & f_{k-1,2} & \cdots & f_{k-1,k} \end{bmatrix}. \tag{4.32}$$

This problem can be solved by using standard numerical techniques.

We next show that, when applying the SMPE approach, the generalized eigenvalue problem we have just discovered can also be formulated more simply in terms of the QR factorization of the matrix $\boldsymbol{F}_{n,k}$, which we compute when implementing the SMPE approach anyway.

Theorem 4.2 *Let the QR factorization of the matrix* $\boldsymbol{F}_{n,k} = [\boldsymbol{f}_n | \boldsymbol{f}_{n+1} | \cdots | \boldsymbol{f}_{n+k}]$ *be given as*

$$\boldsymbol{F}_{n,k} = \boldsymbol{Q}_k \boldsymbol{R}_k, \quad \boldsymbol{Q}_k \text{ unitary}, \quad \boldsymbol{R}_k \text{ upper triangular},$$

with $\boldsymbol{Q}_k$ *and* $\boldsymbol{R}_k$ *precisely of the forms in* (3.10)–(3.11)*. Then, in the SMPE approach, the* $\zeta_i^{(n,k)}$*,* $i = 1, \ldots, k$*, are also the solution of the generalized eigenvalue problem*

$$\det(\boldsymbol{N}_1 - \zeta \boldsymbol{N}_0) = 0, \tag{4.33}$$

where $\boldsymbol{N}_0$ *is obtained from* $\boldsymbol{R}_k$ *by crossing out the last column and the last row, while* $\boldsymbol{N}_1$ *is obtained from* $\boldsymbol{R}_k$ *by crossing out the first column and the last row, that is,*

$$\boldsymbol{N}_0 = \boldsymbol{R}_{k-1} = \begin{bmatrix} r_{00} & r_{01} & \cdots & r_{0,k-1} \\ & r_{11} & \cdots & r_{1,k-1} \\ & & \ddots & \vdots \\ & & & r_{k-1,k-1} \end{bmatrix} \tag{4.34}$$

and

$$\boldsymbol{N}_1 = \begin{bmatrix} r_{01} & r_{02} & \cdots & r_{0,k-1} & r_{0k} \\ r_{11} & r_{12} & \cdots & r_{1,k-1} & r_{1k} \\ & \ddots & \ddots & \vdots & \vdots \\ & & \ddots & \vdots & \vdots \\ & & & r_{k-1,k-1} & r_{k-1,k} \end{bmatrix}. \tag{4.35}$$

Proof We start by noticing that

$$\boldsymbol{M}_0 = \boldsymbol{F}^*_{n,k-1}\boldsymbol{F}_{n,k-1}, \quad \boldsymbol{M}_1 = \boldsymbol{F}^*_{n,k-1}\boldsymbol{F}_{n+1,k-1}.$$

Invoking now the that $\boldsymbol{F}_{n,k-1} = \boldsymbol{Q}_{k-1}\boldsymbol{R}_{k-1}$, we have

$$\boldsymbol{M}_0 = (\boldsymbol{Q}_{k-1}\boldsymbol{R}_{k-1})^*\boldsymbol{Q}_{k-1}\boldsymbol{R}_{k-1} = \boldsymbol{R}^*_{k-1}\boldsymbol{R}_{k-1} = \boldsymbol{R}^*_{k-1}\boldsymbol{N}_0. \tag{4.36}$$

Next, by the fact that

$$\boldsymbol{F}_{n+1,k-1} = [\boldsymbol{Q}_{k-1}|\boldsymbol{q}_k]\left[\frac{\boldsymbol{N}_1}{r_{kk}\boldsymbol{e}_k^T}\right], \quad \boldsymbol{e}_k = [0, 0, \ldots, 0, 1]^T \in \mathbb{C}^k,$$

and that $\boldsymbol{Q}^*_{k-1}\boldsymbol{q}_k = \boldsymbol{0}$, we have

$$\boldsymbol{M}_1 = (\boldsymbol{Q}_{k-1}\boldsymbol{R}_{k-1})^*[\boldsymbol{Q}_{k-1}|\boldsymbol{q}_k]\left[\frac{\boldsymbol{N}_1}{r_{kk}\boldsymbol{e}_k^T}\right] = \boldsymbol{R}^*_{k-1}[\boldsymbol{I}_{k\times k}|\boldsymbol{0}]\left[\frac{\boldsymbol{N}_1}{r_{kk}\boldsymbol{e}_k^T}\right] = \boldsymbol{R}^*_{k-1}\boldsymbol{N}_1. \tag{4.37}$$

Substituting (4.36) and (4.37) in (4.30), and invoking the fact that $\boldsymbol{R}_{k-1}$ is square and nonsingular, we obtain (4.33). □

5 Computational aspects of the new Prony-type methods

We now summarize the computational aspects of the methods suggested by the Montessus- and König-type convergence theories presented in Theorem 4.1 for the vector-valued rational approximations $\boldsymbol{s}_{n,k}$ summarized in Section 4.2. With the sequence of vectors $\{\boldsymbol{f}_m\}$ as in (4.1)–(4.2), to approximate the first k of the ζ_i and the corresponding $\boldsymbol{a}_i$, we proceed as follows:

1. **Determination of the** u_j
   - *When* $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_k$ *are linearly independent:*
     Input the vectors $\boldsymbol{f}_m$, $m = n, n+1, \ldots, n+k$.
     - Solve the (usually inconsistent) $N \times k$ linear system in (4.11) for $u_0, u_1, \ldots, u_{k-1}$ by least squares as in (4.12) (using QR factorization of the matrix $\boldsymbol{F}_{n,k}$). Set $u_k = 1$. This is the SMPE approach.
     - Choose linearly independent vectors $\boldsymbol{g}_1, \ldots, \boldsymbol{g}_k$ and form the $k \times k$ linear system in (4.14), and solve it for $u_0, u_1, \ldots, u_{k-1}$. Set $u_k = 1$. This is the SMMPE approach.
   - *When* $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_k$ *are linearly dependent:*
     Input the vectors $\boldsymbol{f}_m$, $m = n, n+1, \ldots, n+2k-1$.
     Choose a nonzero vector $\boldsymbol{g}$ and form the $k \times k$ linear system in (4.14), and solve it for $u_0, u_1, \ldots, u_{k-1}$. Set $u_k = 1$. This is the STEA approach.
2. **Computation of the approximations** $\zeta_i^{(n,k)}$ **to** ζ_i, $i = 1, \ldots, k$
   With the u_j determined, compute the approximations $\zeta_i^{(n,k)}$ to the ζ_i as the zeros of the polynomial $u(\zeta) = \sum_{j=0}^k u_j\zeta^j$.

3. **Computation of the approximations $\boldsymbol{a}_i^{(n,k)}$ to $\boldsymbol{a}_i$, $i = 1, \ldots, k$**
   With the u_j and the $\zeta_i^{(n,k)}$ available, compute the approximations $\boldsymbol{a}_i^{(n,k)}$ to the $\boldsymbol{a}_i$, $i = 1, \ldots, k$, via

$$\boldsymbol{a}_i^{(n,k)} = -\left[z^{n-1} \frac{\sum_{p=0}^{k} h_{p,k}(z) \boldsymbol{f}_{n+p}}{\sum_{j=0}^{k} (k-j) u_j z^{k-j-1}} \right]\Bigg|_{z=1/\zeta_i^{(n,k)}}, \quad h_{p,k}(z) = \sum_{j=p}^{k} u_j z^{k-j+p}. \tag{5.1}$$

6 Numerical examples

In this section, we provide two examples that confirm some of the claims made in Theorem 4.1.

Example 6.1 Consider the vector sequence $\{\boldsymbol{f}_m\}$, where $\boldsymbol{f}_m = \sum_{i=1}^{8} \boldsymbol{a}_i \zeta_i^m$, $m = 0, 1, \ldots,$ where

$$\zeta_1 = -1,\ \zeta_2 = -\mathrm{i},\ \zeta_3 = \mathrm{i},\ \zeta_4 = 1,\ \zeta_5 = -1/2,\ \zeta_6 = -\mathrm{i}/2,\ \zeta_7 = \mathrm{i}/2,\ \zeta_8 = 1/2,$$

and

$$\begin{aligned}
\boldsymbol{a}_1 &= [1, 1, 1, 1, 1, 1, 1, 1]^T, \\
\boldsymbol{a}_2 &= [1, -1, 1, -1, 1, -1, 1, -1]^T, \\
\boldsymbol{a}_3 &= [1, 1, -1, -1, 1, 1, -1, -1]^T, \\
\boldsymbol{a}_4 &= [1, -1, -1, 1, 1, -1, -1, 1]^T, \\
\boldsymbol{a}_5 &= [1, 1, 1, 1, -1, -1, -1, -1]^T, \\
\boldsymbol{a}_6 &= [1, -1, 1, -1, -1, 1, -1, 1]^T, \\
\boldsymbol{a}_7 &= [1, 1, -1, -1, -1, -1, 1, 1]^T, \\
\boldsymbol{a}_8 &= [1, -1, -1, 1, -1, 1, 1, -1]^T.
\end{aligned}$$

Note that the vectors $\boldsymbol{a}_i$ are the consecutive columns of the Hadamard matrix H_8 and hence are mutually orthogonal.[7] Note also that $\zeta_1, \ldots, \zeta_4$ are on the unit circle, whereas $\zeta_5, \ldots, \zeta_8$ are on the circle with radius $1/2$, hence in the interior of the unit circle.

First, we applied the SMPE approach to this example with $k = 8$ as explained in Section 3 and obtained all the ζ_i with close to machine precision.

Next, we applied the SMPE approach with $k = 4$ and $n = 5, 10, 15, 20$. The results of the computations are given in Table 1. Note that, Theorem 4.1 applies, and, by (4.26) and (4.27), there hold $\lim_{n\to\infty} \zeta_i^{(n,k)} = \zeta_i$ and $\lim_{n\to\infty} \boldsymbol{a}_i^{(n,k)} = \boldsymbol{a}_i$, $i = 1, \ldots, 4$, such that

$$\begin{aligned} \zeta_i^{(n,k)} - \zeta_i &= O(2^{-2n}) \\ \boldsymbol{a}_i^{(n,k)} - \boldsymbol{a}_i &= O(2^{-n}) \end{aligned} \quad \text{as } n \to \infty,\ \text{ since } |\zeta_5/\zeta_i| = 1/2,\ i = 1, \ldots, 4.$$

[7] For Hadamard matrices, see Hall [9], for example.

Table 1 Numerical results for Example 6.1

n	$n=5$	$n=10$	$n=15$	$n=20$
$\lvert\zeta_1-\zeta_1^{(n,4)}\rvert$	$2.29e-04$	$2.24e-07$	$2.18e-10$	$2.13e-13$
$\lVert\boldsymbol{a}_1-\boldsymbol{a}_1^{(n,4)}\rVert_\infty$	$1.70e-02$	$3.58e-04$	$1.53e-05$	$3.48e-07$
$\lvert\zeta_2-\zeta_2^{(n,4)}\rvert$	$2.29e-04$	$2.24e-07$	$2.18e-10$	$2.13e-13$
$\lVert\boldsymbol{a}_2-\boldsymbol{a}_2^{(n,4)}\rVert_\infty$	$1.70e-02$	$3.58e-04$	$1.53e-05$	$3.48e-07$
$\lvert\zeta_3-\zeta_3^{(n,4)}\rvert$	$2.29e-04$	$2.24e-07$	$2.18e-10$	$2.13e-13$
$\lVert\boldsymbol{a}_3-\boldsymbol{a}_3^{(n,4)}\rVert_\infty$	$1.70e-02$	$3.58e-04$	$1.53e-05$	$3.48e-07$
$\lvert\zeta_4-\zeta_4^{(n,4)}\rvert$	$2.29e-04$	$2.24e-07$	$2.18e-10$	$2.13e-13$
$\lVert\boldsymbol{a}_4-\boldsymbol{a}_4^{(n,4)}\rVert_\infty$	$1.70e-02$	$3.58e-04$	$1.53e-05$	$3.48e-07$

Example 6.2 Consider the vector sequence $\{\boldsymbol{f}_m\}$, where $\boldsymbol{f}_m = \sum_{i=1}^{8}\boldsymbol{a}_i\zeta_i^m$, $m = 0, 1, \ldots,$ where

$$\zeta_1=-1,\ \zeta_2=-\mathrm{i},\ \zeta_3=\mathrm{i},\ \zeta_4=1,\ \zeta_5=-1/2,\ \zeta_6=-\mathrm{i}/2,\ \zeta_7=\mathrm{i}/2,\ \zeta_8=1/2,$$

as in Example 6.1, and

$$\begin{aligned}
\boldsymbol{a}_1 &= [1, 1, 1, 1, 1, 1, 1, 1]^T,\\
\boldsymbol{a}_2 &= [2, 2, 2, 2, 2, 2, 2, 2]^T\\
\boldsymbol{a}_3 &= [1, 1/2, 1, 1/2, 1, 1/2, 1, 1/2]^T,\\
\boldsymbol{a}_4 &= [-2, -1, -2, -1, -2, -1, -2, -1]^T,\\
\boldsymbol{a}_5 &= [1, 2, 1, 2, 1, 2, 1, 2]^T,\\
\boldsymbol{a}_6 &= [1, 1, 1, 1, 2, 2, 2, 2]^T,\\
\boldsymbol{a}_7 &= [2, 2, 2, 2, 1, 1, 1, 1]^T,\\
\boldsymbol{a}_8 &= [3, 2, 3, 2, 3, 2, 3, 2]^T.
\end{aligned}$$

Note that the vectors $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_8$ form a linearly dependent set, $\boldsymbol{a}_1$, $\boldsymbol{a}_3$, and $\boldsymbol{a}_6$ being linearly independent. Actually, we have $\boldsymbol{a}_2 = 2\boldsymbol{a}_1$, $\boldsymbol{a}_4 = -2\boldsymbol{a}_3$, $\boldsymbol{a}_5 = 3\boldsymbol{a}_1 - 2\boldsymbol{a}_3$, $\boldsymbol{a}_7 = 3\boldsymbol{a}_1 - \boldsymbol{a}_6$, and $\boldsymbol{a}_8 = \boldsymbol{a}_1 + 2\boldsymbol{a}_3$. Thus, $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_4$ form a linearly dependent set too. Note also that, as in Example 6.1, $\zeta_1, \ldots, \zeta_4$ are on the unit circle, whereas $\zeta_5, \ldots, \zeta_8$ are on the circle with radius $1/2$, hence in the interior of the unit circle.

First, we applied the STEA approach to this example with $k = 8$ as explained in Section 3 and obtained all the ζ_i with close to machine precision.

Next, we applied the STEA approach with $k = 4$ and $n = 5, 10, 15, 20$ also choosing $\boldsymbol{g} = [1, 1, \ldots, 1]^T$. [Note that, with this choice of $\boldsymbol{g}$, $(\boldsymbol{g}, \boldsymbol{a}_i) \neq 0$, for $i = 1, \ldots, 8$, as required in the STEA approach.] The results of the computations are given in Table 2. Note that, Theorem 4.1 applies, and, by (4.25) and (4.27), there hold $\lim_{n\to\infty}\zeta_i^{(n,k)} = \zeta_i$ and $\lim_{n\to\infty}\boldsymbol{a}_i^{(n,k)} = \boldsymbol{a}_i$, $i = 1, \ldots, 4$, such that

$$\left.\begin{aligned}\zeta_i^{(n,k)} - \zeta_i &= O(2^{-n})\\ \boldsymbol{a}_i^{(n,k)} - \boldsymbol{a}_i &= O(2^{-n})\end{aligned}\right.\quad \text{as } n\to\infty,\ \text{since } |\zeta_5/\zeta_i| = 1/2,\ i = 1, \ldots, 4.$$

Table 2 Numerical results for Example 6.2

	$n = 5$	$n = 10$	$n = 15$	$n = 20$
$\lvert\zeta_1 - \zeta_1^{(n,4)}\rvert$	$7.67e-04$	$1.22e-04$	$4.25e-06$	$1.89e-07$
$\lVert\boldsymbol{a}_1 - \boldsymbol{a}_1^{(n,4)}\rVert_\infty$	$1.04e-02$	$2.01e-03$	$9.30e-05$	$8.97e-06$
$\lvert\zeta_2 - \zeta_2^{(n,4)}\rvert$	$3.23e-03$	$2.40e-05$	$3.09e-06$	$3.70e-07$
$\lVert\boldsymbol{a}_2 - \boldsymbol{a}_2^{(n,4)}\rVert_\infty$	$1.76e-02$	$1.02e-03$	$1.29e-04$	$9.43e-06$
$\lvert\zeta_3 - \zeta_3^{(n,4)}\rvert$	$2.20e-04$	$1.29e-04$	$5.81e-06$	$2.93e-07$
$\lVert\boldsymbol{a}_3 - \boldsymbol{a}_3^{(n,4)}\rVert_\infty$	$2.11e-02$	$1.20e-03$	$1.61e-04$	$1.22e-05$
$\lvert\zeta_4 - \zeta_4^{(n,4)}\rvert$	$2.04e-03$	$6.40e-05$	$8.24e-06$	$5.04e-07$
$\lVert\boldsymbol{a}_4 - \boldsymbol{a}_4^{(n,4)}\rVert_\infty$	$6.53e-02$	$3.95e-03$	$2.28e-04$	$1.43e-05$

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