Unitarity of some barycentric rational approximants

Tobias Jawecki^{*} and Pranav Singh[†]

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Abstract

The exponential function maps the imaginary axis to the unit circle and, for many applications, this unitarity property is also desirable from its approximations. We show that this property is conserved not only by the (k, k)-rational barycentric interpolant of the exponential on the imaginary axis, but also by (k, k)-rational barycentric approximants that minimize a linearized approximation error. These results are a consequence of certain properties of singular vectors of Loewner-type matrices associated to linearized approximation errors. Prominent representatives of this class are rational approximants computed by the adaptive Antoulas– Anderson (AAA) method and the AAA–Lawson method. Our results also lead to a modified procedure with improved numerical stability of the unitarity property and reduced computational cost.

Keywords: exponential, unitary, rational approximation, barycentric formula, Loewner matrix, AAA algorithm, AAA–Lawson algorithm 2020 MSC: 15A23 41A20 65D15

1 Introduction

Polynomial and rational approximations to functions have a wide range of applications [Tre19]. Rational approximations have some advantages compared to polynomial approximation [Sal81, SW86, Ber88], two main strengths being strong performance for approximating functions near singularities and on unbounded domains [Tre19].

In the present work we are concerned with (k, k)-rational approximants to the imaginary exponential,

$$r(x) = \frac{p(x)}{q(x)} \approx e^{ix}, \qquad x \in I \subset \mathbb{R},$$
(1.1)

where I is a bounded interval in \mathbb{R} , and p(x) and q(x) are complex polynomials of degree k each. This is closely related to the time integration of ordinary differential equations (ODEs), and different approximations to the exponential function yield different numerical methods for time integration. In this context, boundedness of the underlying rational function on a specific subset of the complex plane results in stable numerical integrators [HW02].

In particular, in context of the application specified in (1.1), i.e. the approximation of the exponential function on an interval on the imaginary axis, the main advantage of rational approximation over polynomial approximation is that there exist rational approximants that satisfy the unitarity property,

$$|r(x)| = 1, \qquad x \in \mathbb{R}. \tag{(\star)}$$

Unitarity of the rational approximants to the imaginary exponential has strong benefits for ODEs with a skew-Hermitian structure [HLW06]. The requirement for unitarity (\star) often arises in the context of equations of quantum mechanics [Lub08, Fao12], for instance.

^{*}Institute for Theoretical Physics, Vienna University of Technology, Vienna, Austria, tobias.jawecki@tuwien.ac.at †Department of Mathematical Sciences, University of Bath, Bath, United Kingdom, ps2106@bath.ac.uk

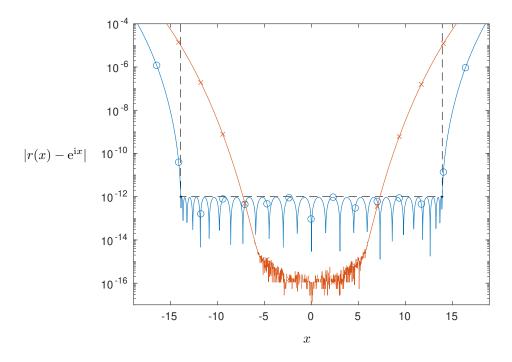


Figure 1: This figure shows the error in two different rational approximations to the imaginary exponential. The error of the diagonal Padé approximant of degree 13 is marked by the symbol (×), while the symbols (\circ) mark the error of a rational approximant generated by the AAA–Lawson method. Namely, the AAA–Lawson method is applied to approximate the imaginary exponential on the interval [-13.9, 13.9] using a (13, 13)-rational function. The error of the AAA–Lawson method is less than 10^{-12} uniformly on the interval, and this error bound is illustrated by a dashed line.

An important class of (k, k)-rational approximants which satisfy the unitarity property (\star) are (diagonal) Padé approximants [BGM96]. Padé approximants have a high order of accuracy around the origin. However, being Taylor based and thus asymptotic in nature, they prove inadequate when a more uniform accuracy over the interval I in (1.1) is desired, or other interpolation properties have to be satisfied.

A more flexible approximation is provided by rational fitting algorithms such as the adaptive Antoulas–Anderson (AAA) method [NST18] and the AAA–Lawson method [NT20], which can provide more accuracy over a relevant interval I (or a discrete set of points) than a diagonal Padé approximant of the same degree. For instance, in Figure 1 we find that a (13, 13)-rational approximant produced by the AAA–Lawson algorithm provides uniformly high accuracy (< 10^{-12}) over the interval of interest. While the diagonal Padé approximant of degree 13 has a very high accuracy in the neighborhood of x = 0, its accuracy towards the extremes of the interval is substantially lower (roughly 10^{-5} near x = -13.9, for instance).

In the present paper, we consider (k, k)-rational approximants in barycentric rational representation of three types:

- (i) rational interpolants of e^{ix} at exactly 2k + 1 nodes,
- (ii) rational approximants of e^{ix} that interpolate e^{ix} at k + 1 support nodes and minimize a linearized error at a larger number of so called *test nodes*, and
- (iii) non-interpolatory rational approximants of e^{ix} that minimize a linearized error at test nodes.

In particular, rational approximants produced by the AAA algorithms fall under type (ii). AAA can also generate approximants with uniform accuracy over an interval I by adaptively choosing

(test and support) nodes. Rational approximants generated by the AAA–Lawson algorithm fall under type (iii). The AAA–Lawson algorithm further increases the accuracy of the approximant generated by AAA by iteratively solving re-weighted least-squares problems. Using a barycentric rational representation for the rational approximation yields two benefits. The first advantage of this representation is strong stability properties [FNTB18, Subsection 2.3]. The other advantage is that the rational approximants of types (i)-(iii) can be found by computing a singular value decomposition of a Loewner matrix [Bel70, Ber00] or an expanded Loewner matrix [NT20].

We show that, while being much more flexible, rational approximants of the type (i)–(iii) share an important property with diagonal Padé approximants: Unitarity (\star), which is highly desirable for applications. In contrast, while the rkfit procedure [BG15] can produce rational approximants with an accuracy comparable to the AAA and AAA–Lawson methods, the approximants generated by rkfit are not unitary in general. This makes AAA and AAA–Lawson methods better suited to applications in (1.1).

Outline of the paper. In Section 2 we recall barycentric rational representations and show, in Proposition 1, that rational interpolants that interpolate e^{ix} at a maximal number of distinct nodes – i.e., of type (i) above – are unitary.

In Section 3, we consider an interpolatory barycentric representation, and express a linearized error in terms of a Loewner matrix. In Subsection 3.1, we consider the case where the linearized error is zero. This corresponds to barycentric rational interpolation which falls under type (i), and consequently, unitarity follows from Proposition 1.

The remaining manuscript is concerned with types (ii) and (iii) – i.e., rational approximants that minimize a linearized error. In Subsection 3.2, we consider interpolatory barycentric approximants of type (ii). Specifically, the approximants generated by the AAA method fall in this class. In Proposition 3, Subsection 3.3, we show that approximants in this class are unitary. These results are generalized to the case of a weighted linearized error in Subsection 3.4. In Section 4 we consider approximants in a non-interpolatory barycentric representation – i.e., type (iii) – as used in the AAA–Lawson method. Unitarity for such approximants is shown in Proposition 5.

Despite the theoretical unitarity of rational approximants of types (ii) and (iii), due to the finite precision of computer arithmetic, in practice these approximants tend to deviate significantly from unitarity away from the domain of approximation (see Figure 2). To remedy this situation, we describe a slight modification to the original AAA and AAA–Lawson algorithms in Section 5. In particular, our approach replaces complex SVD with real SVD, reducing computational cost, and we resort to a Cayley representation, expressing the numerator as the complex conjugate of the denominator. In particular, as illustrated in Figure 2, the modified algorithms, Algorithm 1 and 2, show unitarity at machine precision even away from the domain of approximation.

In Section 6 we briefly sketch the AAA and AAA–Lawson method to illustrate that unitarity indeed holds for approximants generated by these methods. The unitarity results presented in the present paper are based on certain properties of singular vectors of Loewner-type matrices, which are derived in Appendix A.

2 Barycentric rational representation

In the present work we consider rational approximations to the imaginary exponential function. In particular, we make use of barycentric rational representations of rational functions. Approximants in the representations (2.1) and (2.5) below are topic of Section 3 and 4, respectively.

The following barycentric rational representation relies on distinct support nodes $y_1, \ldots, y_m \in \mathbb{R}$ and coefficients $w_1, \ldots, w_m \in \mathbb{C}^m$. For the imaginary exponential function evaluated at the support nodes we also use the notation $f_j = e^{iy_j}$. In Section 3 we consider barycentric rational representations given by the quotient of partial fractions

$$r(x) = \sum_{j=1}^{m} \frac{f_j w_j}{x - y_j} \Big/ \sum_{j=1}^{m} \frac{w_j}{x - y_j} =: n(x)/d(x).$$
(2.1)

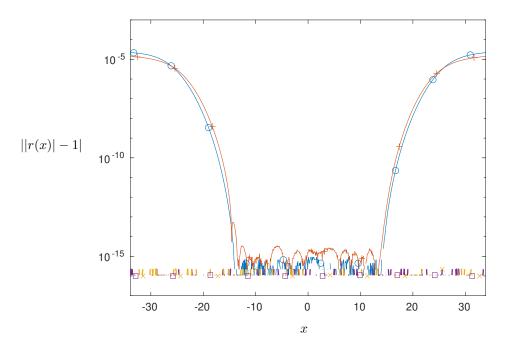


Figure 2: This figure shows the deviation of the unitarity property in computer arithmetic for different barycentric rational approximants. Namely, for the barycentric rational approximants rgenerated by the original (\circ) and modified (\Box) AAA algorithms, and r_b generated by the original (+) and modified (\times) AAA–Lawson algorithms. The modified algorithms are introduced in Section 5. The approximants r and r_b are (14, 14) and (13, 13)-rational functions, respectively, and all approximants are generated to approximate e^{ix} for $x \in [-13.9, 13.9]$ with an approximation error $\leq 10^{-12}$ on this interval. The approximation error of r_b is also illustrated in Figure 1. All of these approximants are unitary in theory, however, in computer arithmetic this property is not exactly preserved when using the original AAA and AAA–Lawson methods. In particular, the deviation in unitarity is below 10^{-14} on the domain of approximation, $x \in [-13.9, 13.9]$, but at x = 35 it is nearly 10^{-5} for the original AAA and AAA–Lawson methods. Unitarity can be maintained uniformly on \mathbb{R} in computer arithmetic by using the modified algorithms – particularly, the deviation of the unitarity property for the modified algorithms is approximately 10^{-16} or exactly zero (not visible in this figure).

The poles of the partial fractions n and d coincide with the support nodes. However, for the function r these singularities are removable. Assuming $w_j \neq 0$, we have the identity

$$r(y_j) = e^{iy_j}, \quad j = 1, \dots, m,$$
 (2.2)

as a limit, so that r interpolates the imaginary exponential at the support nodes.

In the sequel, the notation (m-1, m-1)-rational function refers to a rational function r = p/q, where p and q are polynomials of degree $\leq m-1$. A function in barycentric rational representation (2.1) with m support nodes corresponds to an (m-1, m-1)-rational function. Let

$$\ell(x) = \prod_{j=1}^{m} (x - y_j)$$

denote the polynomial with zeros located at the poles of the partial fractions n and d. We introduce functions p and q as

$$p(x) := \ell(x)n(x) = \sum_{j=1}^{m} f_j w_j \prod_{k \neq j} (x - y_k), \text{ and}$$

$$q(x) := \ell(x)d(x) = \sum_{j=1}^{m} w_j \prod_{k \neq j} (x - y_k).$$
(2.3)

Indeed, p and q correspond to polynomials of degree $\leq m - 1$. Multiplying the numerator and denominator of the barycentric rational representation r by ℓ , we observe

$$r(x) = \frac{\ell(x) n(x)}{\ell(x) d(x)} = \frac{p(x)}{q(x)},$$
(2.4)

which shows that r is an (m-1, m-1)-rational function.

For non-interpolatory approximants in Section 4 we also consider barycentric rational representations

$$r_b(x) = \sum_{j=1}^m \frac{\alpha_j}{x - y_j} \Big/ \sum_{j=1}^m \frac{\beta_j}{x - y_j},$$
(2.5)

where $\alpha_1, \ldots, \alpha_m \in \mathbb{C}$ and $\beta_1, \ldots, \beta_m \in \mathbb{C}$ denote coefficients, and $y_1, \ldots, y_m \in \mathbb{R}$ denote support nodes. In the case of $\alpha_j = f_j w_j$ and $\beta_j = w_j$, this representation coincides with (2.1). In contrast to r in (2.1), r_b does not necessarily interpolate e^{ix} at the support nodes (2.2). In particular, this interpolation property does not hold if $\alpha_j \neq f_j \beta_j$. Expanding r_b similar to (2.4), shows that r_b corresponds to an (m-1, m-1)-rational function.

We refer to a rational function r = p/q as *irreducible* if the polynomials p and q have no common zeros. Furthermore, the *poles* of r refer to the zeros of q. These terms are used in an equivalent manner for a rational function given in barycentric rational representation.

We proceed with some general results concerning (m-1, m-1)-rational interpolations to the imaginary exponential function. Similar results are specified for barycentric rational interpolation in Subsection 3.2.

General remarks on interpolation by (m-1, m-1)-rational functions. For an (m-1, m-1)-rational function r = p/q, the numerator and denominator polynomials are of degree $\leq m-1$ and have m coefficients each. However, the resulting rational function only has 2m-1 free parameters (this result can be observed via partial fraction decomposition). It is natural to consider (m-1, m-1)-rational functions to interpolate the imaginary exponential at 2m-1 given nodes in a general setting. At this point we assume that such a rational interpolation function exists and is irreducible, for further details we refer to [Bel70, Section 2]. The following proposition shows unitarity for this class of rational interpolants.

Proposition 1. Let r be an irreducible (m-1, m-1)-rational function, and let $\theta_1, \ldots, \theta_{2m-1} \in \mathbb{R}$ be distinct nodes such that r satisfies the interpolation property

$$r(\theta_j) = e^{i\theta_j}, \quad j = 1, \dots, 2m - 1.$$
 (2.6)

Then r has no poles on the real axis, and satisfies

$$|r(x)| = 1, \quad for \ x \in \mathbb{R}. \tag{(\star)}$$

A proof of this proposition is provided in Appendix B.

3 Interpolatory rational approximation and Loewner matrices

We proceed to consider rational approximants of e^{ix} in barycentric rational representation (2.1). In the present section, we consider (m-1, m-1)-rational approximants where m is fixed. Approximants of a moderate degree are favourable due to various reasons, e.g., computational cost. Furthermore, a certain approximation accuracy over a given interval or discrete set of nodes is desirable in practice. Due to limitations of the methods discussed in the present work, our focus is on the discrete case. This includes discretized intervals, e.g., [NST18, NT20]. We introduce the notation $x_1, \ldots, x_n \in \mathbb{R}$ for the *test nodes*, over which the rational approximant r needs to approximate e^{ix} ,

$$r(x_k) \approx e^{ix_k}, \quad k = 1, \dots, n, \tag{3.1}$$

with a prescribed accuracy. In addition, the interpolation property at the support nodes (2.2) is desirable in an interpolatory setting. In the sequel, we assume that the support nodes $y_1, \ldots, y_m \in \mathbb{R}$ and the test nodes $x_1, \ldots, x_n \in \mathbb{R}$ are disjoint sets of distinct nodes, unless explicitly stated otherwise.

A special case occurs for n = m - 1, i.e., we have *m* given support nodes and m - 1 given test nodes. This yields a total of 2m - 1 nodes, and as remarked at the end of the previous section, rational interpolation is viable in this setting. Similar interpolation problems have been studied earlier in [Bel70, AA86, Ber00]. As a new result, we prove unitarity of such interpolants in Corollary 2 in Subsection 3.1 based on Proposition 1.

If a larger number of test nodes is given (namely, n > m - 1), then interpolation at all test and support nodes is no longer viable in general. In this case, we replace the interpolation property at the test nodes by a near-best approximation property. In particular, we consider barycentric rational approximants that minimize a linearized error over the test nodes, see Subsection 3.2. This approach is also utilized in the AAA method [NST18]. For the case n > m-1, Proposition 1 does not apply due to non-interpolatory nature. However, in Subsection 3.3 we prove that the approximants that minimize the linearized error are unitary – a new result which is based on properties of singular vectors of a re-scaled Loewner matrix.

We remark that the AAA method also includes an outer iteration to determine the support nodes y_1, \ldots, y_m . However, in this paper we show unitarity for arbitrary support nodes, and therefore we may consider them fixed. A sketch of the AAA method is also given in Section 6 further below.

Barycentric rational approximants that minimize a weighted linearized error satisfy similar unitarity properties, as shown in Subsection 3.4. This setting is motivated by [NST18, Subsection 10], and its applications. Weighted problems also appear in [BG15, BG17].

Non-interpolatory near-best approximants using the representation r_b in (2.5) are discussed in Section 4 further below. Approximants therein are related to the AAA–Lawson method [NT20].

We proceed to introduce common notation concerning the Loewner matrix, which is relevant for barycentric rational approximation in the present section.

Loewner matrix. Assuming $y_1, \ldots, y_m \in \mathbb{R}$ are given support nodes and $x_1, \ldots, x_n \in \mathbb{R}$ are given test nodes, we define the Loewner matrix

$$L \in \mathbb{C}^{n \times m}$$
, with $L_{kj} = \frac{\mathrm{e}^{\mathrm{i}x_k} - \mathrm{e}^{\mathrm{i}y_j}}{x_k - y_j}$, (3.2)

 $k \in \{1, ..., n\}, j \in \{1, ..., m\}$. The Loewner matrix can be written as a product of matrices: Let $C \in \mathbb{R}^{n \times m}$ denote the Cauchy matrix

$$C \in \mathbb{R}^{n \times m}$$
, with $C_{kj} = \frac{1}{x_k - y_j}$, (3.3a)

and let S_F and S_f denote the diagonal matrices

$$S_F = \operatorname{diag}\left(e^{\mathrm{i}x_j}\right) \in \mathbb{C}^{n \times n}, \quad \operatorname{and} \quad S_f = \operatorname{diag}\left(e^{\mathrm{i}y_j}\right) \in \mathbb{C}^{m \times m}.$$
 (3.3b)

Then the Loewner matrix can be expressed as

$$L = S_F C - C S_f \in \mathbb{C}^{n \times m}.$$
(3.4)

For the given support nodes, we consider a barycentric rational approximant r(x) = n(x)/d(x) as in (2.1). We consider $w = (w_1, \ldots, w_m)^\top \in \mathbb{C}^m$ to be the vector of the underlying coefficients in (2.1), which have not been specified yet. The matrices in (3.3) satisfy the following identities when applied to w,

$$(S_F Cw)_k = e^{ix_k} \sum_{j=1}^m \frac{w_j}{x_k - y_j} = e^{ix_k} d(x_k), \text{ and,}$$

$$(CS_f w)_k = \sum_{j=1}^m \frac{f_j w_j}{x_k - y_j} = n(x_k), \text{ where } f_j = e^{iy_j}.$$

(3.5)

Making use of the representation (3.4) and the identities (3.5), we conclude

$$(Lw)_k = e^{ix_k} d(x_k) - n(x_k).$$
 (3.6)

3.1 An (m-1, m-1) rational interpolation at 2m-1 nodes

We proceed with an overview on barycentric rational interpolation of e^{ix} at given nodes. Similar interpolation problems are studied earlier in [Bel70, AA86, Ber00] and others. We assume that 2m - 1 distinct nodes are given; specifically, we assume that we are given m support nodes and m - 1 test nodes, i.e., we have the case n = m - 1. For an example concerning interpolation of e^{ix} at preassigned test and support nodes we also refer to [Kno08, Subsection III.B].

In the present setting the Loewner matrix L given in (3.2) has the dimension $m - 1 \times m$. Thus, L has a non-trivial nullspace. Let the vector of coefficients $w = (w_1, \ldots, w_m)^{\top}$ be in the nullspace of L, i.e.,

$$Lw = 0.$$

Then, due to (3.6), the partial fractions n and d satisfy

$$n(x_k) = d(x_k)e^{ix_k}, \quad k = 1, \dots, m-1.$$
 (3.7)

Furthermore, if the resulting barycentric rational approximation r is irreducible, then (3.7) implies

$$r(x_k) = e^{ix_k}, \quad k = 1, \dots, m-1.$$
 (*)

In the following corollary, we summarize the interpolation properties of r, together with a unitarity property which follows Proposition 1.

Corollary 2. Let $y_1, \ldots, y_m \in \mathbb{R}$ and $x_1, \ldots, x_{m-1} \in \mathbb{R}$ be given support and test nodes, respectively, L be the corresponding Loewner matrix (3.2), and let $w = (w_1, \ldots, w_m)^\top \in \mathbb{C}^m$ denote a vector of coefficients that satisfies Lw = 0. Assume $w_j \neq 0$, and assume the generated barycentric rational function r is irreducible. Then r interpolates e^{ix} at the support and test nodes, has no poles on the real axis, and satisfies

$$|r(x)| = 1, \quad x \in \mathbb{R}. \tag{(\star)}$$

Proof. The barycentric rational function r interpolates at the support nodes due to (2.2) and the assumption $w_j \neq 0$. Following (\star) , the choice of w implies that r interpolates at the test nodes. Thus, r interpolates at a total of 2m - 1 distinct nodes. By construction, r is an (m - 1, m - 1)-rational function. Following Proposition 1, the interpolation properties of r imply that r has to no poles on the real axis and is unitary.

In Subsection 3.3 further below, we provide an alternative proof that the interpolant r considered in Corollary 2 is unitary. This involves a Cayley-type representation for r.

3.2 Minimizing a linearized error

We consider test nodes $x_1, \ldots, x_n \in \mathbb{R}$, where, in contrast to the previous subsection, n > m - 1. In the present subsection, we replace the interpolation property at the test nodes by a near-best approximation property. Namely, we aim to minimize a linearized error over the test nodes; a practical approach which is utilized in the AAA method [NST18].

We recall $r(x) = n(x)/d(x) \approx e^{ix}$, and we linearize this approximation property by multiplying by d(x) on both sides,

$$n(x) \approx e^{ix} d(x). \tag{3.8}$$

For the underlying test and support nodes we consider the Loewner matrix $L \in \mathbb{C}^{n \times m}$ as given in (3.2). Let $w = (w_1, \ldots, w_m)^\top \in \mathbb{C}^m$ refer to the vector of coefficients of r as in (2.1). Following (3.6), the entries of Lw evaluate the deviation in (3.8) at the test nodes, and the Euclidean norm of the vector Lw yields

$$||Lw||_2 = \left(\sum_{k=1}^n |e^{ix_k} d(x_k) - n(x_k)|^2\right)^{1/2}.$$
(3.9)

This representation is referred to as the *linearized error*.

We aim to choose coefficients $w = (w_1, \ldots, w_m)^{\top} \in \mathbb{C}^m$ with $||w||_2 = 1$ such that the linearized error (3.9) is minimized, i.e.,

$$w = \arg\min_{u \in \mathbb{C}^m, \|u\|_2 = 1} \|Lu\|_2.$$
(3.10)

Such coefficients are accessible by exploiting the singular value decomposition of the Loewner matrix L. We have the factorization

$$LV = US, \tag{3.11}$$

where $V \in \mathbb{C}^{m \times m}$ and $U \in \mathbb{C}^{n \times m}$ refer to orthonormal bases of right and left singular vectors, respectively, and $S = \text{diag}(\sigma_1, \ldots, \sigma_m) \in \mathbb{R}^{m \times m}$ refers to a diagonal matrix containing singular values of L. We assume the ordering

$$\sigma_1 \geq \ldots \geq \sigma_m \geq 0.$$

A weight vector w which minimizes the linearized error norm as in (3.10) is attained by a right singular vector of L, e.g.,¹ $w = Ve_m$ with $||Lw||_2 = \sigma_m$. In particular, the smallest singular value of L satisfies

$$\sigma_m \leq ||Lu||_2$$
 for any $u \in \mathbb{C}^m$ with $||u||_2 = 1$.

The generated barycentric rational approximation r interpolates at all test nodes if and only if $\sigma_m = 0$. In general we have the case $\sigma_m > 0$, and interpolation at test nodes is not guaranteed. Thus, Proposition 1 does not apply. Nevertheless, unitarity of the barycentric rational approximant which minimizes the linearized error is shown in the following subsection.

¹We use the notation $e_k = (0, \ldots, 0, 1)^\top \in \mathbb{C}^k$.

3.3 A re-scaled Loewner matrix and unitarity

The coefficients of the barycentric rational approximants discussed in the previous subsections correspond to singular vectors of the Loewner matrix $L \in \mathbb{C}^{n \times m}$. This includes the case n = m - 1 in Subsection 3.1; a vector in the nullspace of L can be understood as a singular vector corresponding to the singular value $\sigma_m = 0$.

The Loewner matrix is of the form (3.4), where the Cauchy matrix C given in (3.3a) is a real matrix. Thus, the Loewner matrix satisfies the representation (A.2) in Appendix A, and we can define a re-scaled Loewner matrix,

$$\widehat{L} = -iRLK \in \mathbb{R}^{n \times m}, \tag{3.12a}$$

which is a real matrix as in (A.9), and

$$K = \operatorname{diag}(K_{11}, \dots, K_{mm}) \in \mathbb{C}^{m \times m}, \quad \text{and} \quad R = \operatorname{diag}(R_{11}, \dots, R_{nn}) \in \mathbb{C}^{n \times n}, \tag{3.12b}$$

are diagonal matrices as in (A.4), with entries

$$K_{jj} = \begin{cases} (1 - e^{-iy_j})/|1 - e^{-iy_j}|, & e^{-iy_j} \neq 1 \text{ and,} \\ i, & \text{otherwise,} \end{cases}$$
(3.12c)

and

$$R_{kk} = \begin{cases} (1 - e^{-ix_k})/|1 - e^{-ix_k}|, & e^{-ix_k} \neq 1 \text{ and,} \\ i, & \text{otherwise.} \end{cases}$$
(3.12d)

Following (A.10), we also note the identity

$$\widehat{L} = 2 \operatorname{Im}(RCK^*), \tag{3.13}$$

where Im(X) denotes the matrix of entry-wise imaginary parts of X.

The diagonal matrices R and K are unitary, and thus, the matrices L and \hat{L} are similar up to a complex phase and their singular values coincide. Furthermore, let the singular value decomposition of the matrix $\hat{L} \in \mathbb{R}^{n \times m}$ be given by

$$\widehat{L}\widehat{V} = \widehat{U}S,\tag{3.14}$$

where $\hat{V} \in \mathbb{R}^{m \times m}$ and $\hat{U} \in \mathbb{R}^{n \times m}$ refer to orthonormal bases of right and left singular vectors, respectively, and $S = \text{diag}(\sigma_1, \ldots, \sigma_m) \in \mathbb{R}^{m \times m}$ as in (3.11). We define

$$\widetilde{w} = iK \widetilde{V} e_m. \tag{3.15}$$

As a corollary of Proposition 8 in Appendix A, the vector \tilde{w} is a singular vector of L corresponding to the singular value σ_m , and as a consequence,

$$\|L\widetilde{w}\|_2 = \sigma_m.$$

Let $\tilde{r} = \tilde{n}/\tilde{d}$ denote the barycentric rational approximant with coefficients \tilde{w} . Then \tilde{r} minimizes the linearized error (3.9), since \tilde{w} is the singular vector corresponding to the smallest singular value, σ_m . This also includes the case n = m - 1 with $\sigma_m = 0$, which is discussed in Subsection 3.1.

Let $\widetilde{w} = (\widetilde{w}_1, \ldots, \widetilde{w}_m)$ be given as in (3.15) and $f_j = e^{iy_j}$. Then Proposition 7 in Appendix A implies

$$f_j \widetilde{w}_j = \widetilde{w}_j^*, \quad j = 1, \dots, m. \tag{3.16}$$

As a consequence, the partial fractions \tilde{n} and \tilde{d} satisfy

$$\widetilde{n}(x) = \sum_{j=1}^{m} \frac{f_j \widetilde{w}_j}{x - y_j} = \sum_{j=1}^{m} \frac{\widetilde{w}_j^*}{x - y_j} = \widetilde{d}(x)^*, \quad \text{for } x \in \mathbb{R},$$
(3.17)

and \tilde{r} has the representation

$$\widetilde{r}(x) = \xi(x)^* \xi(x)^{-1}, \quad \text{with } \xi(x) = d(x).$$
(3.18)

Let \tilde{r} be irreducible, then this further implies that \tilde{r} has no poles on the real axis. Furthermore, \tilde{r} is unitary, i.e., it satisfies

$$|\widetilde{r}(x)| = 1, \quad x \in \mathbb{R}. \tag{(\star)}$$

Concerning uniqueness of w in (3.10), we remark that singular vectors are unique up to a complex phase for the *non-degenerate* case, $\sigma_{m-1} > \sigma_m$. If the smallest singular value is degenerate, any normalized linear combination of singular vectors corresponding to σ_m minimizes (3.10), where in addition, each of these singular vector has an arbitrary complex phase.

In the following proposition we consider barycentric rational approximants that minimize the linearized error but do not necessarily have coefficients \tilde{w} .

Proposition 3. Let $x_1, \ldots, x_n \in \mathbb{R}$ and $y_1, \ldots, y_m \in \mathbb{R}$ be given test and support nodes, respectively, with $n \ge m-1$. Assume the smallest singular value of the corresponding Loewner matrix is nondegenerate, i.e., $\sigma_{m-1} > \sigma_m$. Let r(x) = n(x)/d(x) denote the barycentric rational approximant with coefficients w_1, \ldots, w_m such that the linearized error (3.9) is minimized. Furthermore, assume r is irreducible. Then r has no poles on the real axis and satisfies

$$|r(x)| = 1, \quad x \in \mathbb{R}. \tag{(\star)}$$

Proof. The underlying vector of coefficients $w = (w_1, \ldots, w_m)^{\top}$ corresponds to a singular vector of L which is unique up to a complex phase due to σ_m being a non-degenerate. Namely, we have $w = e^{i\phi}\widetilde{w}$ for \widetilde{w} as given in (3.15) and some complex phase $\phi \in \mathbb{R}$. Due to (3.16), the entries of w satisfy $f_j w_j = e^{2i\phi} w_j^*$. Similar to (3.17), this implies $n(x) = e^{2i\phi} d(x)^*$ and we conclude $r(x) = e^{2i\phi} d(x)^* d(x)^{-1}$. Thus, if r is irreducible it has no poles on the real axis, and satisfies |r(x)| = 1 for $x \in \mathbb{R}$.

Remark 4. Proposition 3 does not apply if the smallest singular value of L is degenerate, i.e., $\sigma_m = \sigma_{m-1}$. To clarify this remark we consider the following example. Let V denote the basis of right singular vectors of L, then the vector $w = (e^{i\psi_1}Ve_m + e^{i\psi_2}Ve_{m-1})/\sqrt{2}$ with arbitrary phases $\psi_1, \psi_2 \in \mathbb{R}$ minimizes $||Lw||_2$. Thus, the barycentric rational approximant with coefficients w minimizes the linearized error (3.9). However, this approximant is not necessarily unitary.

On the other hand, the vector \tilde{w} given in (3.15) also satisfies (3.16) in case of σ_m being degenerate, which entails unitarity of the respective barycentric rational approximant even in the degenerate case.

Following Proposition 7 in Appendix A, $\widetilde{w} = iK\widehat{V}\zeta$ for any $\zeta \in \mathbb{R}^m$ satisfies $f_j\widetilde{w}_j = \widetilde{w}_j^*$. Thus, coefficients corresponding to this vector also generate a unitary rational approximant. However, such an approximant does not minimize the linearized error. Similar results hold for $\widetilde{w} = iK\widehat{V}\zeta$ with $\zeta \in i\mathbb{R}^m$.

3.4 Minimizing a weighted linearized error

We proceed to generalize results of the previous subsections by considering barycentric rational approximants of the form (2.1) that minimize a weighted linearized error over the test nodes. In the unweighted case, the deviation in the approximation $r(x) \approx e^{ix}$ at a test node x_k is $r(x_k) - e^{ix_k}$. In the weighted case, we are given weights,

$$\mu_1, \dots, \mu_n > 0, \tag{3.19}$$

and consider a weighted deviation at test nodes,

$$\mu_k^{1/2}(r(x_k) - e^{ix_k}). \tag{3.20}$$

We slightly modify the Loewner matrix (3.2) to include the weights μ_k . Namely, we define

$$L_{\mu} \in \mathbb{C}^{n \times m}$$
 with $(L_{\mu})_{kj} = \frac{\mu_k^{1/2} (\mathrm{e}^{\mathrm{i}x_k} - \mathrm{e}^{\mathrm{i}y_j})}{x_k - y_j}.$

Similar to (3.4), this matrix satisfies the representation

$$L_{\mu} = S_F M - M S_f, \quad \text{with} \quad M = S_{\mu} C \in \mathbb{R}^{n \times m}, \tag{3.21}$$

where C denotes the Cauchy matrix as given in (3.3a) and $S_{\mu} = \text{diag}\left(\mu_{1}^{1/2}, \ldots, \mu_{n}^{1/2}\right) \in \mathbb{R}^{n \times n}$. Similar to (3.6), applying a vector of coefficients $w = (w_{1}, \ldots, w_{m})^{\top} \in \mathbb{C}^{m}$ to the weighted Loewner matrix yields

$$(L_{\mu}w)_k = \mu_k^{1/2} (e^{ix_k} d(x_k) - n(x_k)),$$

where d and n are partial fractions of the respective barycentric rational representation as in (2.1). Thus, we have

$$||L_{\mu}w||_{2} = \left(\sum_{k=1}^{n} \mu_{k} |\mathrm{e}^{\mathrm{i}x_{k}} d(x_{k}) - n(x_{k})|^{2}\right)^{1/2}.$$
(3.22)

This corresponds to a weighted linearized error which is related to the weighted deviation (3.20).

Considering a barycentric rational approximant r(x) = n(x)/d(x) which minimizes (3.22), we let coefficients $w_1, \ldots, w_m \in \mathbb{C}$ of r correspond to a right singular vector of L_{μ} , namely, the right singular vector corresponding to the smallest singular value of L_{μ} . The matrices L and L_{μ} both satisfy the representation (A.2) in Appendix A. Thus, the results of the previous subsections – in particular, Proposition 3 and the Cayley-type representation given in (3.18) – also apply when considering a weighted linearized error.

4 Non-interpolatory rational approximation

In the present section we consider a barycentric rational approximant r_b based on the representation (2.5) that satisfies some accuracy conditions at n test nodes, where n > m - 1. We proceed with a setting similar to Section 3: Let the degree m be fixed, and let $y_1, \ldots, y_m \in \mathbb{R}$ and x_1, \ldots, x_n be given support and test nodes, respectively. In contrast to the barycentric rational approximant r based on the representation (2.1), which is the topic of the previous section, the approximant r_b does not necessarily interpolate at the support nodes. On the other hand, r_b has more coefficients which are free to be chosen such that a higher accuracy at the test nodes can be achieved for this representation. We aim to choose the coefficients of r_b such that a weighted linearized error is minimized in the progress. This approach is motivated by the AAA–Lawson algorithm [NT20]. The AAA-Lawson algorithm runs in two phases. First, the AAA method is applied, which results in an approximant r of the form (2.1), and support nodes y_1, \ldots, y_m . In the second phase, these support nodes are put in the representation r_b in (2.5), and the coefficients $\alpha_1, \ldots, \alpha_m$ and β_1, \ldots, β_m are determined such that a weighted linearized error is minimized. This phase runs iteratively, adapting the weights of the underlying linearized error with each iteration. A similar approach is already suggested in [NST18] and appears in [FNTB18, Section 8] for the approximation of real functions. Focusing on the unitarity of the generated approximant, we assume the support nodes y_1, \ldots, y_m and the weights to be given.

We recall the barycentric representation given in (2.5),

$$r_b(x) = \sum_{j=1}^m \frac{\alpha_j}{x - y_j} \Big/ \sum_{j=1}^m \frac{\beta_j}{x - y_j} =: n_b(x)/d_b(x),$$
(4.1)

where $\alpha_1, \ldots, \alpha_m \in \mathbb{C}$ and $\beta_1, \ldots, \beta_m \in \mathbb{C}$ denote coefficients which have to be chosen to minimize the linearized error. Let

$$\mu_1,\ldots,\mu_n>0$$

denote given weights which represent scaling factors of the deviation in the approximation $r(x) \approx e^{ix}$ at the test nodes,

$$\mu_k^{1/2}(r_b(x_k) - \mathrm{e}^{\mathrm{i}x_k}).$$

In the current setting, r_b does not necessarily interpolate e^{ix} at the support nodes, and it is reasonable to include support nodes in the set of test nodes such that accuracy at the support nodes can also be enforced. Thus, in the present section we allow test nodes to coincide with support nodes.

To derive a weighted linearized error for the barycentric rational approximant $r_b = n_b/d_b$ in (4.1), we first simplify $r_b(x) \approx e^{ix}$ to $n_b(x) \approx e^{ix}d_b(x)$. Evaluated at a test node x_k which is not a support node, we consider the linearized deviation

$$\mu_k^{1/2}(n_b(x_k) - e^{ix_k} d_b(x_k)).$$
(4.2a)

If the test node x_k is also a support node, there is an index j_k such that $x_k = y_{j_k}$, and the representation r_b as given in (4.1) can not be evaluated at $x = x_k$ in a direct manner due to the presence of the partial fractions $\frac{\alpha_{j_k}}{x-y_{j_k}}$ and $\frac{\beta_{j_k}}{x-y_{j_k}}$. However, in the limit $x \to x_k$ we attain

$$\lim_{x \to x_k} r_b(x) = \alpha_{j_k} / \beta_{j_k}$$

and (4.2a) is replaced by

$$\mu_k^{1/2}(\alpha_{j_k} - e^{ix_k}\beta_{j_k}), \quad \text{for } x_k = y_{j_k}.$$
(4.2b)

The deviations in (4.2) can be represented as a matrix-vector product of an expanded Loewner matrix with the coefficient vectors $\alpha = (\alpha_1, \ldots, \alpha_m)^\top \in \mathbb{C}^m$ and $\beta = (\beta_1, \ldots, \beta_m)^\top \in \mathbb{C}^m$. We introduce a modified Cauchy matrix $C' \in \mathbb{R}^{n \times m}$ as follows.

• Let k be an index with $x_k \notin \{y_1, \ldots, y_m\}$. Then we define the k-th row of C' analogously to the k-th row of the Cauchy matrix C in (3.3). This yields

$$(C'\alpha)_k = \sum_{j=1}^m \frac{\alpha_j}{x_k - y_j} = n_b(x_k), \text{ and } (C'\beta)_k = \sum_{j=1}^m \frac{\beta_j}{x_k - y_j} = d_b(x_k).$$
 (4.3a)

• Otherwise, for an index k with $x_k \in \{y_1, \ldots, y_m\}$ we have an index j_k such that $x_k = y_{j_k}$, and we define the k-th row of C' by

$$C'_{kj} = \begin{cases} 1, & \text{for } j = j_k, \text{ and} \\ 0, & \text{for } j \in \{1, \dots, m\} \setminus \{j_k\}, \end{cases} \text{ for } k, j_k \text{ with } x_k = y_{j_k}.$$

For this index k, the matrix-vector products in (4.3a) yield

$$(C'\alpha)_k = \alpha_{j_k}, \text{ and } (C'\beta)_k = \beta_{j_k}.$$
 (4.3b)

Furthermore, let $S_F \in \mathbb{C}^{n \times n}$ denote the diagonal matrix with diagonal entries e^{ix_k} as in (A.1), and let $M = S_{\mu}C' \in \mathbb{R}^{n \times m}$ where $S_{\mu} = \text{diag}\left(\mu_1^{1/2}, \ldots, \mu_n^{1/2}\right) \in \mathbb{R}^{n \times n}$. The matrix-vector products $M\alpha$ and $M\beta$ can be evaluated similar to (4.3). For the concatenated vector $\gamma = [\alpha; \beta] \in \mathbb{C}^{2m}$ we have

$$([M| - S_F M]\gamma)_k = \begin{cases} \mu_k^{1/2} (n_b(x_k) - e^{ix_k} d_b(x_k), & x_k \notin \{y_1, \dots, y_m\} \text{ and,} \\ \mu_k^{1/2} (\alpha_{j_k} - e^{ix_k} \beta_{j_k}), & x_k = y_{j_k} \text{ for some } j_k, \end{cases}$$
(4.4a)

where $[M| - S_F M]$ is to be understood as the $n \times 2m$ complex matrix obtained by concatenating the $n \times m$ matrices M and $-S_F M$. The Euclidean norm of $[M| - S_F M]\gamma$ quantifies the deviations (4.2) over the test nodes (which may include support nodes) and is also referred to as linearized error in the present section.

In the following, we consider barycentric rational approximants r_b that attain a minimal linearized error. Namely, the vector $\gamma = [\alpha; \beta] \in \mathbb{C}^{2m}$, where α and β refer to the coefficients of r_b , satisfies

$$\gamma = \arg\min_{v \in \mathbb{C}^{2m}, \|v\|_2 = 1} \left\| [M| - S_F M] v \right\|_2.$$
(4.4b)

Similar to the coefficient vector w in (3.10), the vector γ in (4.4b) is accessible using a singular value decomposition of the matrix $[M| - S_F M] \in \mathbb{C}^{n \times 2m}$.

We proceed with some auxiliary properties of right singular vectors of $[M|-S_FM]$. These results are given in detail in Appendix A.1. Let $R = \text{diag}(R_{11}, \ldots, R_{nn}) \in \mathbb{C}^{n \times n}$ be given as in (A.4) in Appendix A, i.e.,

$$R_{kk} = \begin{cases} (1 - e^{-ix_k})/|1 - e^{-ix_k}|, & e^{-ix_k} \neq 1 \text{ and,} \\ i, & \text{otherwise,} \end{cases}$$
(4.5)

and let

$$\widehat{B} = [\operatorname{Re}(R)M| - \operatorname{Im}(R)M] \in \mathbb{R}^{n \times 2m},$$
(4.6)

where $\operatorname{Re}(R)$ and $\operatorname{Im}(R)$ refer to the matrices of entry-wise real and imaginary parts of R, respectively. The matrix \widehat{B} satisfies (A.18) in Appendix A.1 with $\Theta = RM$. Let $\widehat{V}_B \in \mathbb{R}^{2m \times 2m}$ denote a real orthonormal basis of right singular vectors of \widehat{B} as in (A.21), and let

$$\widehat{\gamma} = \widehat{V}_B e_{2m} \in \mathbb{R}^{2m}, \quad \widehat{\gamma} = [\widehat{\alpha}; \widehat{\beta}], \tag{4.7a}$$

denote a right singular vector of \hat{B} corresponding to the smallest singular value of \hat{B} . We introduce the vector

$$\widetilde{\gamma} = \frac{1}{\sqrt{2}} \begin{pmatrix} \widehat{\alpha} + i\widehat{\beta} \\ \widehat{\alpha} - i\widehat{\beta} \end{pmatrix} \in \mathbb{C}^{2m}, \quad \widetilde{\gamma} = [\widetilde{\alpha}; \widetilde{\beta}],$$
(4.7b)

which corresponds to the vector $\tilde{\gamma}$ in (A.24) in Appendix A.1. Following Corollary 10 in Appendix A.1, $\tilde{\gamma}$ satisfies (4.4b), and we have the identity

$$\widetilde{\alpha}_j = \widetilde{\beta}_j^*, \quad j = 1, \dots, m.$$
(4.7c)

Thus, the barycentric rational representation $\tilde{r}_b = \tilde{n}_b/\tilde{d}_b$ with coefficients $\tilde{\alpha}$ and $\tilde{\beta}$ minimizes the linearized error, and \tilde{n}_b and \tilde{d}_b satisfy

$$\widetilde{n}_b(x) = \sum_{j=1}^m \frac{\widetilde{\alpha}_j}{x - y_j} = \sum_{j=1}^m \frac{\widetilde{\beta}_j^*}{x - y_j} = \widetilde{d}_b(x)^*, \quad \text{for } x \in \mathbb{R}.$$
(4.8)

As a consequence, we have the Cayley-type representation

$$\widetilde{r}_b(x) = \xi(x)^* \xi(x)^{-1}, \quad \text{with } \xi(x) = \widetilde{d}_b(x),$$

$$(4.9)$$

and for the case that \tilde{r}_b is irreducible, this implies that \tilde{r}_b has no poles on the real axis and

$$|\tilde{r}_b(x)| = 1, \quad x \in \mathbb{R}. \tag{(\star)}$$

If the smallest singular value of $[M| - S_F M]$ is non-degenerate, then a similar result carries over to any barycentric rational approximant that minimizes the respective linearized error.

Proposition 5. Let the smallest singular value of $[M|-S_FM]$ be non-degenerate, and let $\gamma = [\alpha; \beta]$ satisfy (4.4b). Assume the generated barycentric rational approximant r_b is irreducible. Then r_b has no poles on the real axis and satisfies

$$|r_b(x)| = 1, \quad x \in \mathbb{R}. \tag{(\star)}$$

Proof. For the case that the smallest singular value of $[M| - S_F M]$ is non-degenerate, coefficients α and β that satisfy (4.4b) correspond to $\alpha = e^{i\phi}\tilde{\alpha}$ and $\beta = e^{i\phi}\tilde{\beta}$ for a phase $\phi \in \mathbb{R}$, and $\tilde{\alpha}$ and $\tilde{\beta}$ as given in (4.7b). Due to (4.7c), we have $\alpha_j = e^{2i\phi}\beta_j^*$ for $j = 1, \ldots, m$. Similar to (4.8), this yields $n_b(x) = e^{2i\phi}d_b(x)^*$ for n_b and d_b given in (4.1). Thus, the zeros of d_b and n_b located on the real axis coincide. Together with the assumption that $r_b = n_b/d_b$ is irreducible, this entails that r_b has no poles on the real axis. Furthermore, we have $|r_b(x)| = 1$ for $x \in \mathbb{R}$.

Considering the restriction to a non-degenerate case in Proposition 5, we also refer to Remark 4 in the previous section.

Remark 6. Analogously to the barycentric rational approximant \tilde{r}_b with coefficients corresponding to $\tilde{\gamma}' = Q\hat{V}_B\zeta \in \mathbb{C}^{2m}$ (with Q and \hat{V}_B as in Proposition 9 in Appendix A.1) with $\zeta \in \mathbb{R}^{2m}$ or $\zeta \in \mathbb{R}^{2m}$ is unitary as well. This also holds true when singular values of $[M| - S_F M]$ are degenerate.

5 Advantages of Cayley-type representations

In the present section we give some remarks concerning the computation of the interpolatory and non-interpolatory approximants introduced in the previous sections. We have shown the unitarity property (*) for approximants which minimize linearized errors in the previous sections. The coefficients of the respective barycentric rational approximants are unique up to a complex phase. In practice, we suggest computing coefficients using the re-scaled Loewner matrix $\hat{L} \in \mathbb{R}^{n \times m}$ (3.12a) instead of the original Loewner matrix $L \in \mathbb{C}^{n \times m}$ in the context of the AAA method, or the modified Loewner-type matrix $\hat{B} \in \mathbb{R}^{n \times 2m}$ (4.6) instead of $[M| - S_F M] \in \mathbb{C}^{n \times 2m}$ in the context of the AAA–Lawson method. Furthermore, we suggest utilizing a Cayley-type representation of the rational approximant. These modifications can be implemented for the AAA and AAA–Lawson methods [NST18, NT20], as illustrated in Algorithm 1 and 2 below, which gives some advantages in terms of computational cost and numerical stability of the unitarity property.

We first consider the interpolatory case and the approximant \tilde{r} (3.18) of the representation (2.1) with coefficients $\tilde{w}_1, \ldots, \tilde{w}_m$ as given in (3.15).

- (i) The coefficients $\tilde{w}_1, \ldots, \tilde{w}_m$ can be computed via a singular value decomposition of the rescaled Loewner matrix \hat{L} using real arithmetic. This typically reduces computational cost compared with the original AAA algorithm, which uses a singular value decomposition of a complex Loewner matrix.
- (ii) Exploiting the Cayley-type representation $\tilde{r} = \xi^* \xi^{-1}$ reduces computational cost when \tilde{r} has to be evaluated, or zeros and poles of \tilde{r} are required. In particular, the zeros of \tilde{r} are the complex conjugate of its poles.
- (iii) The complex phases of the coefficients $\tilde{w}_1, \ldots, \tilde{w}_m$ originate from applying the complex diagonal matrix iK in (3.15) on the real vector $\hat{V}e_m$. Thus, these complex phases are exact up to machine precision, and are not affected by errors that occur from the underlying singular value decomposition. As a consequence, the identity $f_j w_j = w_j^*$ (3.16) is true up to machine precision. This results in an improved numerical stability on the unitarity of \tilde{r} compared to r. For the deviation of the unitarity property of approximants generated by the original and modified AAA algorithms in computer arithmetic, see Figure 2.
- (iv) In a degenerate or close to degenerate case, the approximant \tilde{r} with coefficients $\tilde{w}_1, \ldots, \tilde{w}_m$ remains unitary, see also Remark 4.

In Algorithm 1, we illustrate the modifications (i) and (ii) for the AAA method, which yields a modified AAA algorithm utilizing (i)–(iv). This algorithm is based on a simplified version of **aaa.m** in the **chebfun** package [DHT14]. Note that only a minimal version of the original AAA algorithm – adequate for illustrating the modification based on the Cayley-type representation – is described

in the present work. For further details of AAA we refer to [NST18], and the short summary given in Section 6.

Algorithm 1 Pseudocode for a modified AAA algorithm generating a barycentric rational approximant of e^{ix} . See aaa.m in the chebfun package and [NST18, Fig. 4.1] for the original code in full detail.

Require: $(x_1, \ldots, x_N), m_{\max}, n_{\text{lawson}}$ 1: $F \leftarrow (e^{ix_1}, \dots, e^{ix_N})$ 1: $F \leftarrow (e^{-1}, \dots, e^{-ix})$ 2: $R \leftarrow diag((1 - e^{-ix_1})/|1 - e^{-ix_1}|, \dots, (1 - e^{-ix_N})/|1 - e^{-ix_N}|)$ 3: for all j with $(e^{-ix_j} == 1)$ set $R_{jj} = i$ \triangleright the matrix R as in (3.12d) 4: $r \Leftarrow \operatorname{mean}(F) \cdot (1, \dots, 1) \in \mathbb{C}^N$ 5: **for** $m = 1, ..., m_{\max}$ **do** $j \Leftarrow \arg \max(|F - r|)$ 6: 7: $y_m \Leftarrow x_j$ $f_m \leftarrow F_j$ $k_m \leftarrow R_{jj}$ remove x_j from the list of test nodes, i.e., $x \leftarrow (x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_{N-m+1})$ 8: 9:10: and remove the respective columns of C and F and entries of R $c_{\text{new}} \leftarrow \left(\frac{1}{x_1 - y_m}, \dots, \frac{1}{x_{N-m} - y_m}\right)^\top$ $C \leftarrow [C \mid c_{\text{new}}]$ 11:12: $K \Leftarrow \operatorname{diag}(k_1, \ldots, k_m)$ 13: $\widehat{L} \leftarrow 2\operatorname{Im}(R \cdot C \cdot \operatorname{conj}(K)) \in \mathbb{R}^{(N-m) \times m}$ \triangleright the re-scaled Loewner matrix (3.13). 14: $(\widehat{U}, S, \widehat{V}) \Leftarrow \mathtt{svd}(\widehat{L})$ 15: $\widetilde{w} \Leftarrow i K \widehat{V} e_m \in \mathbb{C}^m$ \triangleright see (3.15) 16: $\xi \Leftarrow C \cdot \widetilde{w}$ 17: $r \leftarrow (\xi_1^*/\xi_1, \dots, \xi_{N-m}^*/\xi_{N-m})$ $\triangleright = (r(x_1), \dots, r(x_{N-m}))$ using $r = \xi^* / \xi$ 18: 19: **end for** \triangleright run Algorithm 2 20: if $n_{\text{lawson}} > 0$ then $\widetilde{w} \Leftarrow \min(x = (x_1, \dots, x_{N-m}), y = (y_1, \dots, y_m), n_{\text{lawson}})$ 21:22: end if 22. end if 23. return $x \mapsto r(x) = \sum_{j=1}^{m} \frac{\tilde{w}_{j}^{*}}{x-y_{j}} / \sum_{j=1}^{m} \frac{\tilde{w}_{j}}{x-y_{j}} \qquad \triangleright \text{ using the Cayley-type representation (3.18)}$ \triangleright for the case $n_{\text{lawson}} > 0$ with $\widetilde{w}_j = \widetilde{\beta}_j$, the generated r(x) corresponds to (4.9)

We proceed to discuss advantages of utilizing the non-interpolatory approximant \tilde{r}_b in (4.9) with the coefficients $\tilde{\alpha}_1, \ldots, \tilde{\alpha}_m$ and $\tilde{\beta}_1, \ldots, \tilde{\beta}_m$ given in (4.7). The following points are similar to (i)-(iv) above.

- (i-b) The coefficients $\tilde{\alpha}_1, \ldots, \tilde{\alpha}_m$ and $\tilde{\beta}_1, \ldots, \tilde{\beta}_m$ can be computed via a singular value decomposition of $\hat{B} \in \mathbb{R}^{n \times 2m}$ (4.6) using real arithmetic. This reduces computational cost compared with the original AAA–Lawson algorithm which uses the singular value decomposition of the complex matrix $[M| - S_F M] \in \mathbb{C}^{n \times 2m}$.
- (ii-b) Exploiting the Cayley-type representation $\tilde{r}_b = \xi^* \xi^{-1}$ given in (4.9) reduces computational cost when \tilde{r}_b has to be evaluated, or zeros and poles of \tilde{r}_b are required.
- (iii-b) Using the formula (4.7) to compute the coefficients $\tilde{\alpha}_1, \ldots, \tilde{\alpha}_m$ and $\tilde{\beta}_1, \ldots, \tilde{\beta}_m$ helps avoid errors on the complex phases of the coefficients, which can occur during the computation of a singular value decomposition of $[M] - S_F M$. This also results in an improved numerical stability on the unitarity of \tilde{r}_b compared to r_b . For the deviation of the unitarity property of approximants generated by the original and modified AAA–Lawson algorithms in computer arithmetic, see Figure 2.
- (iv-b) In a degenerate or close to degenerate case, the approximant \tilde{r}_b with coefficients $\tilde{\alpha}_1, \ldots, \tilde{\alpha}_m$ and $\tilde{\beta}_1, \ldots, \tilde{\beta}_m$ remains unitary, see also Remark 6.

In Algorithm 2, we illustrate the modifications (i-b) and (ii-b) for the minimax iteration which is part of the AAA-Lawson method. This algorithm is based on a simplified version of **aaa.m** in the **chebfun** package [DHT14]. In combination with Algorithm 1 (and ' $n_{\text{lawson}} > 0$ '), Algorithm 2 yields a modified version of the AAA-Lawson algorithm utilizing (i-b)-(iv-b).

Algorithm 2 Pseudocode for a modified *minimax* iteration which is called by Algorithm 1 to generate coefficients of a near-best rational approximant of e^{ix} . This algorithm is based on **aaa.m** in the **chebfun** package and yields a modified version of the AAA-Lawson method.

Require: $x = (x_1, ..., x_n), y = (y_1, ..., y_m), n_{\text{lawson}}$ 1: $N \Leftarrow n + m$ 2: $x \leftarrow (x_1, \ldots, x_n, y_1, \ldots, y_m) \in \mathbb{R}^N$ \triangleright include support nodes to the set of test nodes 3: $\mu \leftarrow (1, \ldots, 1) \in \mathbb{R}^N$ 4: $F \Leftarrow (e^{ix_1}, \dots, e^{ix_N})$ 5: $R \leftarrow \operatorname{diag}((1 - e^{-ix_1})/|1 - e^{-ix_1}|, \dots, (1 - e^{-ix_N})/|1 - e^{-ix_N}|)$ 6: for all j with $(e^{-ix_j} == 1)$ set $R_{jj} = i$ \triangleright the matrix R as in (4.5) 7: $C \Leftarrow 0 \in \mathbb{C}^{N \times m}$ \triangleright the Cauchy matrix C', some test and support nodes coincide 8: for $j = 1, \dots, n$ do 9: $C_{j,:} \leftarrow \left(\frac{1}{x_j - y_1}, \dots, \frac{1}{x_j - y_m}\right)$ 10: end for 11: for j = 1, ..., m do $C_{n+j,j} \Leftarrow 1$ 12: 13: end for 14: $A \leftarrow [\operatorname{Re}(R) \cdot C] - \operatorname{Im}(R) \cdot C] \in \mathbb{R}^{N \times 2m}$ 15: for $steps = 1, \ldots, n_{\text{lawson}}$ do $S_{\mu} \Leftarrow \operatorname{diag}(\sqrt{\mu_1}, \ldots, \sqrt{\mu_N})$ 16: $(\widehat{U}, \widehat{S}, \widehat{V}) \Leftarrow \mathtt{svd}(S_{\mu} \cdot A)$ \triangleright svd of $\widehat{B} = S_{\mu} \cdot A$, see (4.6) 17: $\widehat{\gamma} \Leftarrow \widehat{V} e_{2m} \in \mathbb{R}^{2m}$ 18: \triangleright see (4.7a) $\widetilde{\beta} = (\widetilde{\beta}_1, \dots, \widetilde{\beta}_m)$ with $\widetilde{\beta}_j \leftarrow (\widehat{\gamma}_j - i\widehat{\gamma}_{j+m})/\sqrt{2}$ $\xi \leftarrow 0 \in \mathbb{C}^N$ 19: ▷ see (4.7b) 20: for $\ell = 1, \ldots, n$ do 21: $\xi_{\ell} \Leftarrow \sum_{j=1}^{m} \frac{\widetilde{\beta}_j}{x_{\ell} - y_j}$ 22:end for 23:for $\ell = 1, \ldots, m$ do 24: $\xi_{n+\ell} \Leftarrow \beta_\ell$ 25:end for 26: $r \leftarrow (\xi_1^*/\xi_1, \dots, \xi_N^*/\xi_N)$ 27: \triangleright using the Cayley-type representation (4.9) $\varepsilon \Leftarrow F - r$ 28: $\mu \leftarrow (\mu_1|\varepsilon_1|,\ldots,\mu_N|\varepsilon_N|)$ 29: $\mu \Leftarrow \mu / \|\mu\|_\infty$ 30: 31: end for 32: return $\widetilde{\beta} = (\widetilde{\beta}_1, \dots, \widetilde{\beta}_m)$

6 Unitarity of AAA and AAA–Lawson methods

We briefly sketch the AAA and AAA–Lawson algorithms to illustrate that Proposition 3 and 5 apply in these settings, respectively. This shows unitarity (\star) of the generated approximants.

6.1 Unitarity of the AAA method

Let us consider the application of the AAA algorithm [NST18] to the approximation of e^{ix} . This algorithm aims to generate a barycentric rational approximant r using the representation (2.1)

which is accurate at a given set of test nodes $x_1, \ldots, x_n \in \mathbb{R}$, while the degree *m* of the approximant is increased in an iterative manner. The initial iteration step uses an approximant with a single support node, i.e., m = 1, and, the iteration proceeds as follows.

- (a) The number of support nodes, i.e., the degree m, is increased. In particular, the test node for which the previously computed approximant yields the largest deviation from e^{ix} is added to the set of support nodes, and removed as a test node.
- (b) The coefficients $w_1, \ldots, w_m \in \mathbb{C}$ are computed such that the linearized error is minimized (3.10), which generates a new approximant.
- (c) Accuracy conditions are tested for the new approximant. If error tolerances are satisfied, AAA returns the generated approximant. Otherwise, the iteration proceeds with (a).

In addition, *Froissart doublets* can be detected by AAA. If Froissart doublets occur, specific nodes are removed from the set of support and test nodes, and the coefficients are re-computed by minimizing the linearized error for the new sets of nodes.

Due to the fact that coefficients w_1, \ldots, w_m minimize the linearized error as in (3.10), Proposition 3 applies and shows that the generated approximant has no poles on the real axis and is unitary. This requires further conditions of Proposition 3 to hold true. Namely, the smallest singular value of the underlying Loewner matrix has to be non-degenerate, and the generated approximant has to be irreducible.

6.2 Unitarity of the AAA–Lawson method

We proceed to sketch the application of the AAA–Lawson method, which is introduced in [NT20], to the approximation of e^{ix} . We show that Proposition 5 applies in this case and the generated approximant is unitary. The AAA–Lawson method first runs the AAA method, which is summarized in the previous subsection. This returns a set of support nodes $y_1, \ldots, y_m \in \mathbb{R}$ which is fixed for the following procedure. The algorithm then proceeds to find a near-best approximant using the barycentric rational representation r_b given in (2.5). This requires determining proper coefficients $\alpha_1, \ldots, \alpha_m$ and β_1, \ldots, β_m , which is done in an iterative procedure as summarized below. In contrast to the AAA algorithm, the support nodes are included in the set of test nodes in the AAA–Lawson algorithm.

As an initial iteration step, the algorithm introduces weights $\mu_1, \ldots, \mu_n = 1$.

- (a) The coefficients α_j and β_j are computed to satisfy (4.4), where μ_k in (4.4a) refers to the current weights. This provides an approximant r_b which minimizes the respective weighted linearized error.
- (b) A new set of weights is computed. Namely, we update the weights μ_k to $\mu_k |r_b(x_k) e^{ix_k}|$. In addition, weights are normalized. Then the iteration proceeds with (a) until a given number of iteration runs are done or other conditions are satisfied.

In any case, the coefficients of the generated approximant r_b minimize a weighted linearized error as in (4.4) and Proposition 5 applies in this setting, assuming further conditions given therein hold true. This shows the approximant generated by the AAA–Lawson method has no poles on the real axis and is unitary.

Appendix

A Properties of singular vectors of Loewner-type matrices

In the present section we show properties of singular vectors of matrices related to the Loewner matrix (3.4). Namely, we first consider matrices of the type (A.2) introduced below. In Subsection A.1 below, we consider singular vectors of matrices which are related to expanded Loewner

matrices, namely, matrices of the type (A.15) introduced below. Similar to previous sections, we let $x_1, \ldots, x_n \in \mathbb{R}$ and $y_1, \ldots, y_m \in \mathbb{R}$ denote given test and support nodes, respectively, and we define the diagonal matrices

$$S_F = \operatorname{diag}\left(e^{\mathrm{i}x_j}\right) \in \mathbb{C}^{n \times n}, \quad \operatorname{and} \quad S_f = \operatorname{diag}\left(e^{\mathrm{i}y_j}\right) \in \mathbb{C}^{m \times m}.$$
 (A.1)

Let $M \in \mathbb{R}^{n \times m}$ be a given real matrix, and let

$$A = S_F M - M S_f \in \mathbb{C}^{n \times m}.$$
(A.2)

The singular value decomposition of A yields the factorization

$$AV = US,\tag{A.3}$$

where $V \in \mathbb{C}^{m \times m}$ and $U \in \mathbb{C}^{n \times m}$ denote orthonormal bases of right and left singular vectors, respectively, and $S = \text{diag}(\sigma_1, \ldots, \sigma_m)$ denotes a diagonal matrix of singular values. For the singular values we assume the ordering

$$\sigma_1 \geq \ldots \geq \sigma_m \geq 0.$$

We proceed with some auxiliary results. Define the diagonal matrices

$$K = \operatorname{diag}(K_{11}, \dots, K_{mm}) \in \mathbb{C}^{m \times m}, \quad \text{and} \quad R = \operatorname{diag}(R_{11}, \dots, R_{nn}) \in \mathbb{C}^{n \times n}, \tag{A.4a}$$

with diagonal entries

$$K_{jj} = \begin{cases} (1 - e^{-iy_j})/|1 - e^{-iy_j}|, & e^{-iy_j} \neq 1 \text{ and,} \\ i, & \text{otherwise,} \end{cases}$$
(A.4b)

where i refers to the imaginary unit, and

$$R_{kk} = \begin{cases} (1 - e^{-ix_k})/|1 - e^{-ix_k}|, & e^{-ix_k} \neq 1 \text{ and,} \\ i, & \text{otherwise.} \end{cases}$$
(A.4c)

The diagonal entries of K satisfy

$$e^{iy_j}K_{jj} = e^{iy_j}\frac{(1 - e^{-iy_j})}{|1 - e^{-iy_j}|} = \frac{e^{iy_j} - 1}{|1 - e^{-iy_j}|} = -K_{jj}^*, \text{ for } e^{-iy_j} \neq 1.$$
(A.5a)

The identity $e^{iy_j}K_{jj} = -K_{jj}^*$ directly holds true for the case $e^{-iy_j} = 1$ with $K_{jj} = i$. In a similar manner, diagonal entries of R satisfy

$$e^{ix_k}R_{kk} = e^{ix_k}\frac{(1 - e^{-ix_k})}{|1 - e^{-ix_k}|} = \frac{e^{ix_k} - 1}{|1 - e^{-ix_k}|} = -R_{kk}^*, \text{ for } e^{-ix_k} \neq 1.$$
 (A.5b)

and this identity also holds true for the case $e^{-ix_k} = 1$. In matrix form, (A.5a) implies

$$S_f K = -K^*, \tag{A.6a}$$

where S_f refers to the diagonal matrix with diagonal entries e^{iy_j} . In a similar manner, (A.5b) implies

$$S_F R = -R^*, \tag{A.6b}$$

where S_F refers to the diagonal matrix with diagonal entries e^{ix_k} .

Proposition 7. Let $\zeta \in \mathbb{R}^m$ be given, then a vector $w = iK\zeta$ with $w = (w_1, \ldots, w_m)^\top \in \mathbb{C}^m$ satisfies

$$f_j w_j = w_j^*, \quad for \ \ j = 1, \dots, m,$$
 (A.7)

where $f_j = e^{iy_j}$.

Proof. Rewriting both sides of (A.7) in matrix-vector form, and substituting w therein yields

$$f_j w_j = (S_f w)_j = (\mathbf{i} S_f K \zeta)_j, \quad \text{and} \quad w_j^* = (-\mathbf{i} K^* \zeta)_j,$$

where S_f denotes the diagonal matrix with diagonal entries f_j . Making use of the identity (A.6a), we conclude (A.7).

We proceed to rewrite the matrix-product RAK: Substituting (A.2) for A and making use of (A.6), we observe

$$R(S_FM - MS_f)K = -R^*MK + RMK^* = 2i\operatorname{Im}(RMK^*) \in i\mathbb{R}^{n \times m},$$
(A.8)

where Im(X) denotes the entry-wise imaginary part of a matrix X. We define

$$\widehat{A} = -iRAK \in \mathbb{R}^{n \times m}.$$
(A.9)

The matrix \widehat{A} is real due to (A.8). In particular, (A.8) shows

$$\widehat{A} = 2 \operatorname{Im}(RMK^*). \tag{A.10}$$

The matrices A and \widehat{A} are similar up to a complex phase, and thus, these matrices share the same set of singular values. Let the singular value decomposition of the matrix $\widehat{A} \in \mathbb{R}^{n \times m}$ be given by

$$\widehat{A}\widehat{V} = \widehat{U}S,\tag{A.11}$$

where $\widehat{V} \in \mathbb{R}^{m \times m}$ and $\widehat{U} \in \mathbb{R}^{n \times m}$ denote orthonormal bases of right and left singular vectors, respectively, and the diagonal matrix $S \in \mathbb{R}^{m \times m}$ consists of the singular values of \widehat{A} . Here, Sin (A.11) is the same as that in (A.3), since A and \widehat{A} are similar. For the real matrix \widehat{A} , sets of real right and left singular vectors are accessible and unique up to a change of signs. The bases of left and right singular vectors are orthonormal, i.e., the matrices \widehat{V} and \widehat{U} are unitary²,

$$\widehat{V}^* \widehat{V} = I$$
 and $\widehat{U}^* \widehat{U} = I.$ (A.12)

Proposition 8. The matrices

$$U = -R^* \widehat{U} \in \mathbb{C}^{n \times m}, \quad and \quad V = iK \widehat{V} \in \mathbb{C}^{m \times m}$$
(A.13)

correspond to orthonormal bases of right and left singular vectors of A, respectively.

Proof. The matrices K and R given in (A.4) satisfy

$$R^*R = I, \quad \text{and} \quad K^*K = I. \tag{A.14}$$

As in (A.12), the matrices \hat{U} and \hat{V} are unitary, and together with (A.14) this implies that U and V as given in (A.13) are unitary.

With (A.13), we have

$$\widehat{U} = -RU$$
, and $\widehat{V} = -iK^*V$

Substituting these identities in (A.11), we arrive at

$$iR^*\widehat{A}K^*V = US$$

Substituting the identity (A.9) therein, we conclude that V and U given in (A.13) satisfy a singular value decomposition of A which completes the proof. \Box

²In this paper we consider orthogonality with respect to the Hermitian inner product $\langle v, u \rangle = v^* u$, so that a matrix with (complex) orthonormal columns is unitary. This is to be distinguished from the more common convention where orthogonal matrices are defined with respect to the inner product $\langle v, u \rangle = v^T u$, and real orthogonal matrices are distinct from unitary matrices.

A.1 Auxiliary results for the non-interpolatory case

We recall some previously introduced notation. In the present section, the matrix $M \in \mathbb{R}^{n \times m}$ refers to a given real matrix and $S_F \in \mathbb{C}^{n \times n}$ denotes the diagonal matrix with diagonal entries e^{ix_k} as in (A.1). Our main interest in the present subsection lies in the singular value decomposition of

$$[M] - S_F M] \in \mathbb{C}^{n \times 2m} \tag{A.15}$$

and properties of its right singular vectors.

Let R be the diagonal matrix given as in (A.4). With $RS_F = -R^*$ as given in (A.6b), we have

$$R[M| - S_F M] = [RM|R^*M].$$

Due to R being unitary, the matrices $[M| - S_F M]$ and $[RM|R^*M]$ share the same set of right singular vectors and singular values.

We proceed to show results in a slightly more general setting: For a given matrix $\Theta \in \mathbb{C}^{n \times m}$, we consider the matrix

$$B = [\Theta|\operatorname{conj}(\Theta)] \in \mathbb{C}^{n \times 2m},$$

where $\operatorname{conj}(\Theta)$ denotes the matrix with complex conjugate entries of Θ . Considering the present work, the case $\Theta = RM$ with $B = [RM|R^*M]$ is the most relevant one.

For the singular value decomposition of B we write

$$BV_B = U_B S_B,\tag{A.16}$$

where $S_B = \text{diag}(\sigma_1, \ldots, \sigma_{2m}) \in \mathbb{R}^{2m \times 2m}$ is the diagonal matrix of singular values, and $V_B \in \mathbb{C}^{2m \times 2m}$ and $U_B \in \mathbb{C}^{n \times 2m}$ are the matrices of singular vectors. For the singular values we assume the ordering

$$\sigma_1 \geq \ldots \geq \sigma_{2m} \geq 0.$$

To determine properties of the entry-wise complex phases of the singular vectors of B, we proceed to introduce the unitary transformation³

$$Q = \frac{1}{\sqrt{2}} \begin{pmatrix} I_m & \mathrm{i}I_m \\ I_m & -\mathrm{i}I_m \end{pmatrix} \in \mathbb{C}^{2m \times 2m}, \quad \text{which satisfies} \quad Q^*Q = I_{2m}. \tag{A.17}$$

Furthermore, we introduce the matrix $\widehat{B} \in \mathbb{R}^{n \times 2m}$ as

$$\widehat{B} = \left[\operatorname{Re}(\Theta) \mid -\operatorname{Im}(\Theta)\right] \in \mathbb{R}^{n \times 2m}.$$
(A.18)

The matrices B and \hat{B} satisfy the relation

$$\widehat{B} = \frac{1}{\sqrt{2}} BQ. \tag{A.19}$$

Thus, the matrices B and \hat{B} share the same set of singular values up to a factor $\sqrt{2}$. We introduce the matrix

$$\widehat{S}_B = \frac{1}{\sqrt{2}} S_B,\tag{A.20}$$

where S_B refers to the diagonal matrix of singular values of B as in (A.16). The singular value decomposition of the real matrix \hat{B} yields a factorization

$$\widehat{B}\widehat{V}_B = \widehat{U}_B\widehat{S}_B,\tag{A.21}$$

where $\hat{U}_B \in \mathbb{R}^{n \times 2m}$ and $\hat{V}_B \in \mathbb{R}^{2m \times 2m}$ denote real orthonormal bases of left and right singular values, respectively, and \hat{S}_B is given in (A.20).

³The notations I and I_k refer to the identity matrix throughout the present work. Here, I_k explicitly refers to the $k \times k$ -dimensional identity matrix.

We proceed to re-scale \widehat{V}_B by Q to construct a basis of right singular vectors of B. To this end we introduce the matrix

$$\widetilde{V}_B = Q \widehat{V}_B \in \mathbb{C}^{2m \times 2m},\tag{A.22}$$

with $\widehat{V}_B \in \mathbb{R}^{2m \times 2m}$ as in (A.21).

Proposition 9. Let \widehat{S}_B (A.20), $\widehat{U}_B \in \mathbb{R}^{n \times 2m}$ and $\widehat{V}_B \in \mathbb{R}^{2m \times 2m}$ satisfy (A.21), and let $\widetilde{V}_B \in \mathbb{C}^{2m \times 2m}$ be given as in (A.22). Then, \widetilde{V}_B and \widehat{U}_B correspond to orthonormal bases of right and left singular vectors of B, respectively. Namely, according to (A.16) we have the factorization

$$B\widetilde{V}_B = \widehat{U}_B S_B. \tag{A.23}$$

Proof. Substituting (A.19) for \widehat{B} and (A.20) for \widehat{S}_B in the factorization (A.21), we have

$$BQ\widehat{V}_B = \widehat{U}_B S_B.$$

Substituting $\tilde{V}_B = Q\hat{V}_B$ therein we arrive at (A.23). Concerning the unitarity of \tilde{V}_B and \hat{U}_B , we recall that \hat{V}_B and \hat{U}_B refer to orthonormal bases of right and left singular values of \hat{B} . Thus, \hat{U}_B is unitary, and with Q being an unitary transformation, we also conclude that $\tilde{V}_B = Q\hat{V}_B$ is unitary.

The right singular vector of B corresponding to the smallest singular value is of some interest in previous sections. In the setting of Proposition 9, the vectors $\hat{\gamma} = \hat{V}_B e_{2m} \in \mathbb{R}^{2m}$ and $\tilde{\gamma} = \tilde{V}_B e_{2m} \in \mathbb{C}^{2m}$ yield singular vectors of \hat{B} and B, respectively, each corresponding to the smallest singular value of the respective matrix. With $\tilde{V}_B = Q\hat{V}_B$ we have $\tilde{\gamma} = Q\hat{\gamma}$. Substituting (A.17) for Q and writing $\hat{\gamma} = [\hat{\alpha}; \hat{\beta}] \in \mathbb{R}^{2m}$, we arrive at

$$\widetilde{\gamma} = \frac{1}{\sqrt{2}} \begin{pmatrix} I_m & \mathrm{i}I_m \\ I_m & -\mathrm{i}I_m \end{pmatrix} \begin{pmatrix} \widehat{\alpha} \\ \widehat{\beta} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \widehat{\alpha} + \mathrm{i}\widehat{\beta} \\ \widehat{\alpha} - \mathrm{i}\widehat{\beta} \end{pmatrix} \in \mathbb{C}^{2m}.$$
(A.24)

Corollary 10. Let $B = [RM|R^*M]$, i.e., the case $\Theta = RM$. Let $\tilde{\gamma} = \tilde{V}_B e_{2m} \in \mathbb{C}^{2m}$ where \tilde{V}_B satisfies Proposition 9. We also write $\tilde{\gamma} = [\tilde{\alpha}; \tilde{\beta}]$ with $\tilde{\alpha} = (\tilde{\alpha}_1, \ldots, \tilde{\alpha}_m)^\top \in \mathbb{C}^m$ and $\tilde{\beta} = (\tilde{\beta}_1, \ldots, \tilde{\beta}_m)^\top \in \mathbb{C}^m$. Then,

• the vector $\widetilde{\gamma}$ attains the minimum

$$\left\| [M| - S_F M] \widetilde{\gamma} \right\|_2 = \min_{v \in \mathbb{C}^{2m}, \|v\|_2 = 1} \left\| [M| - S_F M] v \right\|_2, \tag{A.25}$$

and

• its entries satisfy

$$\widetilde{\alpha}_j = \widetilde{\beta}_j^*, \quad j = 1, \dots, m. \tag{A.26}$$

Proof. As stated previously in the present subsection, the set of right singular vectors and singular values of the matrices $[M| - S_F M]$ and $B = [RM|R^*M]$ coincide. Following Proposition 9, the vector $\tilde{\gamma}$ corresponds a right singular vector of B corresponding to the singular value σ_{2m} , which is the smallest singular value of B. This carries over to $[M| - S_F M]$, thus, $\|[M| - S_F M]\tilde{\gamma}\|_2 = \sigma_{2m}$ minimizes (A.25). Following (A.24), we have

$$\widetilde{\alpha} = (\widehat{\alpha} + i\widehat{\beta})/\sqrt{2}, \text{ and } \widetilde{\beta} = (\widehat{\alpha} - i\widehat{\beta})/\sqrt{2},$$

where $\widehat{\alpha}, \widehat{\beta} \in \mathbb{R}^m$ correspond to $\widehat{\gamma} = \widehat{V}_B e_{2m}$. This implies the identity (A.26).

B Unitarity of (m-1, m-1) rational interpolation at 2m-1 nodes

Proof of Proposition 1. The interpolation property (2.6) for r = p/q implies

$$|p(\theta_j)| = |q(\theta_j)|, \quad j = 1, \dots, 2m - 1.$$

Applying Proposition 11 given below, we conclude |p(x)| = |q(x)| for $x \in \mathbb{R}$. As a consequence, the sets of real zeros of p and q coincide, and assuming that p and q have no common zeros, we further conclude that r has no poles on the real axis. These properties entail |r(x)| = 1 for $x \in \mathbb{R}$ which completes the proof.

The proof of Proposition 1 requires the following auxiliary result.

Proposition 11. Let p and q denote polynomials of degree $\leq m-1$, and let $\theta_1, \ldots, \theta_{2m-1} \in \mathbb{R}$ be distinct points with

$$|p(\theta_j)| = |q(\theta_j)|, \quad j = 1, \dots, 2m - 1.$$
 (B.1)

Then,

$$|p(x)| = |q(x)|, \quad x \in \mathbb{R}.$$
(B.2)

Proof. Define $\chi = |p|^2 - |q|^2$. Due to p and q being polynomials of degree $\leq m-1$ and x being real, the functions $|p(x)|^2$ and $|q(x)|^2$ conform to polynomials of degree $\leq 2m-2$. Thus, $\chi \colon \mathbb{R} \to \mathbb{R}$ is a polynomial of degree $\leq 2m-2$. The identity (B.1) implies that χ has 2m-1 distinct zeros on the real axis, and as a consequence, χ is the zero polynomial which further implies (B.2).

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