LEAST SQUARES RATIONAL APPROXIMATION*

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Abstract. Rational approximation appears in many contexts throughout science and engineering, playing a central role in linear systems theory, special function approximation, and many others. There are many existing methods for solving the rational approximation problem, from fixed point methods like the Sanathanan-Koerner iteration and Vector Fitting, to partial interpolation methods like Adaptive Anderson Antoulas (AAA). While these methods can often find rational approximations with a small residual norm, they are unable to find optimizers with respect to a weighted \( \ell_2 \) norm with a square dense weighting matrix. Here we develop a nonlinear least squares approach constructing rational approximations with respect to this norm. We explore this approach using two parameterizations of rational functions: a ratio of two polynomials and a partial fraction expansion. In both cases, we show how we can use Variable Projection (VARPRO) to reduce the dimension of the optimization problem. Although this nonlinear least squares approach often converge to suboptimal local minimizers, we find this can be largely mitigated by initializing the algorithm using the poles of the AAA algorithm applied to the same data. This combination of initialization and nonlinear least squares enables us to construct rational approximants using dense and potentially ill-conditioned weight matrices such as those that appear as a step in new \( \mathcal{H}_2 \) model reduction algorithm recently developed by the authors.

Key words. rational approximation, nonlinear least squares, variable projection

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1. Introduction. Rational approximation plays a role in several applications in science and engineering; for example, rational approximations are a critical component in \( \mathcal{H}_2 \)-model reduction [6], can be used in special function computation [9, sec. 9.2], and many others [23, Chap. 23]. Generally posed, the goal of rational approximation is to mimic a function \( f : \mathbb{C} \to \mathbb{C} \) by a degree \((m, n)\) rational function \( r(z) : \mathbb{C} \to \mathbb{C} \)

\[
f \approx r \in \mathcal{R}_{m,n}(\mathbb{C}) := \left\{ \frac{p}{q} : p \in \mathcal{P}_m(\mathbb{C}), \ q \in \mathcal{P}_n(\mathbb{C}) \setminus \{0\} \right\}
\]

where \( \mathcal{P}_m(\mathbb{C}) \) denotes the set of polynomials of degree \( m \) with coefficients in \( \mathbb{C} \). There are several senses in which we might seek to construct a rational approximation. For example, Padé approximation [2] chooses \( r \) to match the first \( m + n \) derivatives of \( f \) at some point \( \hat{z} \in \mathbb{C} \):

\[
r \in \mathcal{R}_{m,n}(\mathbb{C}) \quad \text{such that} \quad f^{(k)}(\hat{z}) = r^{(k)}(\hat{z}) \quad \forall k = 0, 1, \ldots, m + n.
\]

In special function approximation, the goal is often to construct a minimax rational approximation [8] that minimizes the maximum mismatch over a set \( \mathcal{Z} \subset \mathbb{C} \):

\[
\text{minimize } \sup_{r \in \mathcal{R}_{m,n}(\mathbb{C})} \sup_{z \in \mathcal{Z}} |f(z) - r(z)|.
\]

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In this paper we seek to construct a least squares rational approximation over a discrete set of $N$ points $\mathcal{Z} \subset \mathbb{C}$ in a weighted $\ell_2$ norm with a dense weight matrix $W \in \mathbb{C}^{N \times N}$:

\begin{equation}
\text{minimize} \| W \{ f(\mathcal{Z}) - r(\mathcal{Z}) \} \|_2^2 \quad \text{where} \quad f(\mathcal{Z}) := \begin{bmatrix} f(z_1) \\ \vdots \\ f(z_N) \end{bmatrix}, \quad r(\mathcal{Z}) := \begin{bmatrix} r(z_1) \\ \vdots \\ r(z_N) \end{bmatrix}.
\end{equation}

Our motivation for studying this weighted least squares rational approximation comes from a new $H_2$ model reduction algorithm developed by the authors [15] where a rational approximation of this form appears at each step of the algorithm with a weight matrix $W$ that is the inverse matrix square root of a Cauchy matrix. Existing algorithms for rational approximation cannot incorporate this non-diagonal weight matrix, leading us to develop an algorithm to solve (1.4) based standard nonlinear least squares techniques.

There are a variety of existing algorithms for rational approximation. For example as discussed in subsection 2.1, the Loewner framework of Anderson and Antoulas [1] for rational interpolation has been extended by Nakatsukasa, Sète, and Trefethen [18] to rational approximation problem in the Adaptive Anderson-Antoulas (AAA) algorithm; however this does not minimize the nonlinear least squares problem (1.4) and does not incorporate a weighting matrix. Similarly, as discussed in subsection 2.2, there are fixed point methods such as the Sanathanan-Koerner (SK) iteration [20] and the Vector Fitting algorithm of Gustavsen and Semlyen [12] which have fixed points nearby minimizers of the nonlinear least squares problem (1.4). These methods can incorporate a diagonal weighting matrix, but the dense weighting matrix $W$ required for the $H_2$ model reduction problem.

One might ask: why not use nonlinear least squares methods? To use this approach, we first need to specify a parameterization for the rational approximant $r$. Although there are many potential parameterizations, here we focus on two: a polynomial parameterization and a partial fraction parameterization. In the polynomial parameterization, we define $r$ by the coefficients $a \in \mathbb{C}^m$ and $b \in \mathbb{C}^n$ of the numerator and denominator polynomials expressed in bases $\{ \phi_k \}_{k=0}^m \subset \mathcal{P}_m(\mathbb{C})$ and $\{ \psi_k \}_{k=0}^n \subset \mathcal{P}_n(\mathbb{C})$

\begin{equation}
r(z; a, b) := \frac{p(z; a)}{q(z; b)} = \frac{\sum_{k=0}^m a_k \phi_k(z)}{\sum_{k=0}^n b_k \psi_k(z)}.
\end{equation}

In a partial fraction parameterization, which is limited to degree $(m,n)$ rational functions where $m \geq n-1$, we define $r$ as a sum of degree $(0,1)$ rational functions described by their poles $\lambda \in \mathbb{C}^n$ and residues $\rho \in \mathbb{C}^n$ plus an additional set of polynomial coefficients $c \in \mathbb{C}^{m-n}$

\begin{equation}
r(z; \lambda, \rho, c) := \sum_{k=1}^n \frac{\rho_k}{z - \lambda_k} + \sum_{k=0}^{m-n} c_k \varphi_k(z).
\end{equation}

Sections 3 and 4 provide formulas for the residual and Jacobian for these two parameterizations. However, with either parameterization the challenge with this approach is spurious local minima. As illustrated in Figure 1.1 when optimizing in the partial fraction parameterization starting from different initialization, the algorithm finds different local minimizers. Moreover these minimizers frequently have a larger residual.

\footnote{also spelled Löwner}
Fig. 1.1. Spurious local minima are a significant problem when building a rational approximation via optimization compared to the SK iteration and Vector Fitting described in subsection 2.2. Here each dot shows the normalized residual of rational approximants generated from ten different initializations of each algorithm. Both the SK iteration and Vector Fitting frequently converge to a rational approximant with similar residual norm, whereas our optimization approach strongly depends on the starting rational function. However, by initializing using AAA, denoted by crosses +, we are able to mitigate this dependence on initial condition and find a local minimizer that is comparable to that of Vector Fitting. The performance of the SK iteration after $n \geq 18$ is caused by ill-conditioning as illustrated in Figure 2.2. In this example $f$ is the $(1, 1)$ entry of the transfer function of the CD player model [4] evaluated at 1000 points evenly sampled on the imaginary axis between $-10^3 \Im$ and $10^3 \Im$.

norm than the solutions generated by the Vector Fitting and the SK iteration before $n > 14$ when numerical instability emerges. This explains the relative infrequency with which rational approximation is treated using an optimization approach; we are only aware of one paper by Lefteriu and Antoulas where this approach is briefly described [17]. One approach to mitigate the issue of spurious local minima is to find an effective initialization. Here we advocate using the AAA algorithm as an initialization for a standard Gauss-Newton method with a backtracking line search (see, e.g., [19, sec. 10.3]; we use this combination to construct the remainder of our examples. As evidenced in Figure 1.1, coupling this initialization approach with Gauss-Newton yields better minimizers than random initialization, and the residual norm associated with these optimizers is comparable to that generated by Vector Fitting.

Additionally, in this paper we also address how to construct a real rational approximation, where $r$ is a real rational function

$$r \in \mathcal{R}_{m,n}(\mathbb{R}) := \left\{ \frac{p}{q} : p \in \mathcal{P}_m(\mathbb{R}), \ q \in \mathcal{P}_n(\mathbb{R})\backslash\{0\}\right\}$$

where $\mathcal{P}_n(\mathbb{R})$ is the space of degree $n$ polynomials with real coefficients. This constraint is frequently present in model reduction context since the transfer function $f(z) = c^*(Iz - A)^{-1}b$ is a real rational function if $A$, $b$, and $c$ are real. Although imposing this constraint in the polynomial parameterization is straightforward, doing so in the partial fraction expansion requires more care which we discuss in subsection 4.2.

In the remainder of this paper we first describe AAA algorithm, the SK iteration, and Vector Fitting in section 2 and discuss their numerical proprieties. Then
in sections 3 and 4 we derive the residual and Jacobian for the polynomial and partial fraction parameterizations using Variable Projection (VARPRO) [10] to pose the optimization problem only over the nonlinear parameters and also showing how to enforce the constraint that the rational approximant is real. We conclude that due to poor conditioning, the partial fraction parameterization is preferable unless the goal is to build a rational approximation of degree \((m, n)\) where \(m < n - 1\), which can not be expressed in this parameterization. Then in section 5 we provide an example of the effect of imposing the real constraint and evaluate the performance of our algorithm in an example mimicking a step of the projected \(H_2\) algorithm. Finally we discuss extending our optimization approach to vector and matrix valued output data in section 6.

2. Existing Methods for Rational Approximation. In this section we describe two popular classes of algorithms for rational approximation: those based on the Loewner framework originating in the work of Antoulas and Anderson [1], such as the Adaptive Antoulas Anderson (AAA) algorithm [18], and fixed point iterations, such as the Sanathanan-Koerner iteration [20] and Vector Fitting [12]. While these methods are successful in consistently obtaining a rational approximation with a small residual as illustrated in Figure 1.1, none of these methods can incorporate a dense square mass matrix. Moreover, our numerical experiments suggest that that the rational approximations that these methods generate do not satisfy the first order necessary conditions for the least squares rational approximation problem (1.3). In the remainder of this section we will briefly derive each method, illustrating that each method uses a similar trick—multiplying by the denominator of the polynomial, effectively ‘linearizing’ the problem—and discuss how this affects the ability of the algorithm to obtain a least squares estimate. Although these methods do not provide least squares estimates, they are capable of providing rational interpolants (in exact arithmetic) when both \(r\) and \(f\) are degree \((m, n)\) rational functions.

2.1. Loewner Framework. The original work by Anderson and Antoulas presented a technique for determining if a rational interpolant of a specified degree exists and, if so, gave a formula for such a rational interpolant [1, eq. (2.11)]. The central feature of this analysis is a (generalized) Loewner matrix, defined through the input-output pairs \((z_j, f(z_j))\). Although the original derivation permitted interpolation including arbitrary orders of derivatives, here we will describe a simplification for the rational approximation problem called the Adaptive Antoulas Anderson (AAA) algorithm developed by Nakatsukasa, Sète, and Trefethen [18].

A key feature of methods in the Loewner framework is splitting the sample points \(Z\) into two disjoint sets: \(\hat{Z} := \{\tilde{z}_k\}_{k=0}^n \subset Z\) and \(\tilde{Z} := \{\tilde{z}_k\}_{k=n}^N \subset Z\) where \(\hat{Z} \cup \tilde{Z} = Z\). Then, the key step this approach takes to relax the rational approximation problem is forcing the rational approximant \(r\) to interpolate at the values in \(\tilde{Z}\). This results in a simple method to find the rational partial-interpolant—namely, the singular value decomposition (SVD).

To see this in the context of the AAA algorithm, we express the rational approximation \(r\) using the same Lagrange basis for numerator and denominator, restricting this approach to building degree \((n, n)\) rational approximants. In particular, we will use a Lagrange basis expressed in an unweighted barycentric form [3, eq. (3.3)] with Lagrange nodes \(\{\tilde{z}_j\}_{j=0}^n = Z\) where we will later force interpolation:

\[
\phi_k(z) = (z - \tilde{z}_k)^{-1} \ell(z), \quad \ell(z) = \prod_{k=0}^{n} (z - \tilde{z}_k)
\]
Hence if we assume

Next, invoking the (suboptimal) assumption that \( r \) interpolates \( f \) on \( \hat{Z} \), we require that (after removing a removable singularity),

Hence if we assume \( b_k \neq 0 \), we can set \( a_k := b_k f(\hat{z}_k) \) yielding an expression for our rational approximant only in terms of \( b \):

This is related to the second form of the barycentric formula [3, eq. (4.2)], where in the case of polynomial approximation \( b_k \) is fixed \( b_k = \prod_{k \neq j}(\hat{z}_k - \hat{z}_j) \); this expression is also called the rational barycentric formula [16, eq. (1.7)].

At this point we still need to find a choice of \( b \) such that \( r \) approximates \( f \) well on the remainder of the points in \( Z \), namely \( \hat{Z} \). Ideally, we would solve the nonlinear least squares problem:

however, this is still a challenging nonlinear least squares problem. Instead, if we multiply through by the denominator, introducing a second modification of the optimization problem, we find that \( b \) now appears linearly in each row

After this modification, we find \( b \) as the smallest singular value of the Loewner matrix \( L \in \mathbb{C}^{(N-n-1) \times (n+1)} \) built from the input output pairs:

The net result of these approximations is an easy approach for finding a rational approximant, but one that is necessary suboptimal with respect to the \( \ell_2 \) norm due to the interpolation condition (2.3) and multiplication by the denominator in (2.6). However, as illustrated in Figure 2.1, this approach will yield increasingly good rational approximants as measured in residual norm with increasing degree, but ones that are outperformed by our optimization based approach for building rational approximants.

One of the important contributions of the AAA algorithm was providing a greedy heuristic for selecting interpolation points, given in Algorithm 2.1. The authors also discuss removing Froissart doublets—poles with either small residues or pole-zero pairs that nearly cancel—an important consideration for the quality of approximation when the norm of the residual becomes small.
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\[ \text{Fig. 2.1. Comparison of the residual } \| f(Z) - r(Z) \|_2 \text{ where the rational approximation } r \text{ is generated by AAA (9) and our optimization approach using a pole residue parameterization described in section 4 (8). The left takes } f \text{ from the CD Player model as described in Figure 1.1. The right takes } f(z) = \tan(256z) \text{ evaluated at 1000 points uniformly on the unit circle following [18, Fig. 6.4].} \]

**Algorithm 2.1 Adaptive Anderson Antoulas (AAA)**

**Input**: Input output pairs \( \{ (z_j, f(z_j)) \}_{j=1}^N \), desired degree approximant \((n, n)\)

**Output**: Rational approximation \( r(z) = \frac{\sum_{k=0}^{n} f(\tilde{z}_k) \psi_k (z - \tilde{z}_k)^{-1}}{\sum_{k=0}^{n} \psi_k (z - \tilde{z}_k)^{-1}} \)

1. Set residual \( r_j \leftarrow f(z_j) \quad j = 1, \ldots, N \);
2. \( \tilde{Z} \leftarrow \mathbb{Z} \);
3. for \( \ell = 0, 1, \ldots, n \) do
   4. \( j \leftarrow \arg \max_j |r_j| \);
   5. Remove \( z_j \) from \( \tilde{Z} \) and place in \( \tilde{Z} \);
   6. Construct the Loewner matrix \([L]_{j,k} \leftarrow (f(\tilde{z}_j) - f(\tilde{z}_k))/(\tilde{z}_j - \tilde{z}_k)\);
   7. Compute SVD: \( U \Sigma V^* \leftarrow L \);
   8. \( b \leftarrow [V]_{\ell, \ell} \);
   9. Compute residual \( r_j \leftarrow \begin{cases} f(z_j) - \frac{\psi_{\ell} f(\tilde{z}_\ell) \psi_{k}(z_j - \tilde{z}_k)^{-1}}{\sum_{k=0}^{n} \psi_{k} (z_j - \tilde{z}_k)^{-1}}, & z_j \in \tilde{Z} \\ 0, & z_j \notin \tilde{Z} \end{cases} \)

2.2. Fixed Point Iterations. An alternative to the Loewner framework are fixed point iterations, such as the Sanathan-Koerner (SK) iteration [20] and Vector Fitting [12, 11]. Both iterations exploit the same trick of multiplying through by the denominator which was seen in (2.6) and, unlike AAA, do not require interpolation at a set of \( n + 1 \) points. Although the SK iteration and Vector Fitting were developed independently, their similar underpinning has been previously discussed by Hendrickx and Dhaene [14]. Here we focus on the numerical features of each algorithm, noting the SK iteration can become ill-conditioned even when using a polynomial basis that is well conditioned, such as a Legendre basis. However, Vector Fitting avoids this fault by working asymptotically in a partial fraction expansion. Although both algorithms can provide good rational approximations, neither satisfy the first order optimality criteria for least squares rational approximation when data \( f(z_i) \) is generated by a function \( f \) not in \( \mathcal{R}_{m,n} \) [22].

2.2.1. The Sanathan-Koerner Iteration. Suppose we are given a basis for the numerator and denominator, \( \{ \phi_k \}_{k=0}^m \) and \( \{ \psi_k \}_{k=0}^n \) and construct the rational
If we define Vandermonde matrices $\Phi \in \mathbb{C}^{N \times m}$ and $f \in \mathbb{C}^{N \times n}$, we can write this optimization problem as

\[
(2.9) \quad \min_{a \in \mathbb{C}^{m+1}, b \in \mathbb{C}^{n+1}} \|f - \text{diag}(\Psi b)^{-1}\Phi a\|_2, \quad [\Phi]_{j,k} := \phi_k(z_j), \quad [\Psi]_{j,k} := \psi_k(z_j),
\]

and $f = [f(z_1), \ldots, f(z_N)]^T$. One common approach to building a rational approximation prior to Sanathanan and Koerner’s 1963 paper was to multiply through by the denominator, as in AAA, yielding a linear least squares problem:

\[
(2.10) \quad \min_{a \in \mathbb{C}^{m+1}, b \in \mathbb{C}^{n+1}} \|\text{diag}(f)\Psi b - \Phi a\|_2.
\]

The key insight of Sanathanan and Koerner was to introduce a weighting to correct for the wrong norm introduced by multiplying through by the denominator. If at step $\ell$, we have coefficients $a^{(\ell)}$ and $b^{(\ell)}$, the next step is chosen by solving a problem weighted by the previous denominator:

\[
(2.11) \quad a^{(\ell+1)}, b^{(\ell+1)} \leftarrow \min_{a \in \mathbb{C}^{m+1}, b \in \mathbb{C}^{n+1}} \|\text{diag}(\Psi b^{(\ell)})^{-1}[\text{diag}(f)\Psi b - \Phi a]\|_2.
\]

Then if $a^{(\ell)} \to a^{(*)}$ and $b^{(\ell)} \to b^{(*)}$, then $a^{(*)}$ and $b^{(*)}$ appear to provide a least squares solution.

There is one additional choice that is left to be made: how to fix the free scaling shared between $a$ and $b$. In the original paper Sanathanan and Koerner, working in the monomial basis, pick the constant term to set to one that $f$ is in the right hand side of the least squares problem. Here we follow a similar approach when $\{\psi_k\}_{k=0}^n$ is an orthogonal basis of increasing degree, such a Legendre polynomials, which in this case yields the step:

\[
(2.12) \quad a^{(\ell+1)}, b^{(\ell+1)} \leftarrow \min_{a \in \mathbb{C}^{m+1}, b \in \mathbb{C}^{n+1}} \|\text{diag}(\Psi b^{(\ell)})^{-1}[f + [\Psi]_{1:n}\{b\}_{1:n} - \text{diag}(f)\Phi a]\|_2;
\]

where $b_0^{(\ell+1)} = \psi_0(0)$. This approach is used in our implementation, given in Algorithm 2.2. Our experiments suggest that changing the normalization changes the fixed points of this algorithm. This particular constraint yielded the best fixed points in terms of residual norm of those we experimented with.

Although this algorithm frequently converges to fixed points, the linear system that is solved to update $a$ and $b$ in (2.12) rapidly becomes ill-conditioned with increasing degree as illustrated in Figure 2.2. This is not a function of the polynomial basis, as we have transformed the Legendre basis to be orthogonal on $[-1000i, 1000i]$ and the condition number of $\Phi$ and $\Psi$ both remain below 10. However, the condition number of base iteration matrix $[-\Phi \quad \text{diag}(f)[\Psi]_{1:n}]$ and that of the scaling $\text{diag}(\Psi b)^{-1}$ grow rapidly, combining in the large condition number seen. This motivates adaptive basis used by Vector Fitting.

\textbf{2.2.2. Vector Fitting.} Vector Fitting uses a similar approach to the SK iteration, but makes two subtle changes, which combined remove the ill-conditioning
The first difference with the SK iteration is that vector fitting uses a Lagrange basis with nodes $\lambda^{(\ell)}$ that change at each iteration:

\begin{align}
\phi_k^{(\ell)}(z) &= (z - \lambda_k^{(\ell)})^{-1} \prod_{k=1}^n (z - \lambda_k^{(\ell)}) \quad k = 1, \ldots, n \\
\psi_0^{(\ell)}(z) &= \prod_{k=1}^n (z - \lambda_k^{(\ell)}) \quad \text{and} \quad \psi_k^{(\ell)} = \phi_k^{(\ell)}(z) \quad k = 1, \ldots, n
\end{align}

(2.13) \hspace{2cm} (2.14)

Then, as in AAA, we take the ratio and canceling the common product, yielding the parameterization

\begin{equation}
\begin{split}
r(z; a, b, \lambda^{(\ell)}) &= \frac{\sum_{k=1}^n a_k \phi_k^{(\ell)}(z)}{\sum_{k=0}^n b_k \psi_k^{(\ell)}(z)} = \frac{\sum_{k=1}^n a_k (z - \lambda_k^{(\ell)})^{-1}}{b_0 + \sum_{k=1}^n b_k (z - \lambda_k^{(\ell)})^{-1}} \\
&= \frac{\sum_{k=1}^n a_k (z - \lambda_k^{(\ell)})^{-1}}{b_0 + \sum_{k=1}^n b_k (z - \lambda_k^{(\ell)})^{-1}} \tag{2.15}
\end{split}
\end{equation}

As with the SK iteration, we multiply through by the denominator to yield a linear
Algorithm 2.3 Vector Fitting

\begin{algorithm}
\textbf{Input}: Input-output pairs \( \{z_j, f(z_j)\}_{j=1}^N \), initial poles \( \lambda_0 \), degree \((m, n)\)
\textbf{Output}: Rational approximation \( r(z) = \sum_{k=1}^{m} \phi_k(z) - \lambda_k^{-1} \sum_{k=1}^{m} c_k \varphi_k(z) \)
\begin{algorithmic}[1]
\For{\( \ell = 0, 1, \ldots \)}
\State Form Cauchy matrix \( [C^{(\ell)}]_{j,k} = (z_j - \lambda_k^{(\ell)})^{-1} \);
\State Form additional polynomial basis: \( \Phi \in \mathbb{C}^{N \times (m-n)} \), \([\Phi]_{j,k} = \varphi_k(z_j)\);
\State Solve \( \begin{bmatrix} a_{(\ell+1)} \\ b_{(\ell+1)} \end{bmatrix} \leftarrow \arg\min_{a, b} \| f - \begin{bmatrix} -C^{(\ell)} & -\Phi \end{bmatrix} \text{diag}(f) C^{(\ell)} \begin{bmatrix} a \\ b \end{bmatrix} \|_2 \);
\State Set \( \lambda_{(\ell+1)} \) to be eigenvalues of \( \text{diag}(\lambda^{(\ell)}) - 1b^T \);
\If{\( \|b\|_2 < \text{tol} \)} \textbf{break}; \EndIf
\EndFor
\State Residues \( \rho \leftarrow [a^{(*)}]_{1:n} \);
\State Coefficients of polynomial terms \( c \leftarrow [a^{(*)}]_{n+1:m+1} \);
\State Poles \( \lambda \leftarrow \lambda^{(*)} \);
\end{algorithmic}
\end{algorithm}

optimization problem,

\[ a^{(\ell+1)}, b^{(\ell+1)} = \arg\min_{a, b} \| \text{diag}(f) \Psi^{(\ell)} b - \Phi^{(\ell)} a \|_2 \]

(2.16)
where \( [\Psi^{(\ell)}]_{j,0} = 1 \), \( [\Psi^{(\ell)}]_{j,k} = (z - \lambda_k^{(\ell)})^{-1} \), \( [\Phi^{(\ell)}]_{j,k} = (z - \lambda_k^{(\ell)})^{-1} \).

As with the SK iteration, we have a free scaling between \( a \) and \( b \). In the original version of vector fitting [12], this was dealt with by fixing \( b_0 = 1 \). In an updated version Gustavsen recommends adding a constraint that the average real part of the denominator is one [11, eq. (8)]:

(2.17)
\[ \sum_{j=1}^{N} \sum_{k=1}^{n} \Re[b_0 + b_k(z_j - \lambda_k^{(\ell)})^{-1}] = N. \]

Unlike the SK iteration, vector fitting iteration (2.16) does not include a scaling by the previous denominator. Instead, after every iteration the Lagrange nodes \( \lambda^{(\ell)} \) are updated to be the roots the denominator polynomial by solving the eigenvalue problem [11, eq. (5)]:

(2.18)
\[ A \mathbf{x}_k = \lambda_k^{(\ell+1)} \mathbf{x}_k, \quad A = \text{diag}(\lambda^{(\ell)}) - 1b_{1:n}^T/b_0 \in \mathbb{C}^{n \times n}. \]

Then, if \( \lambda^{(\ell)} \) converges to \( \lambda^{(*)} \), the denominator coefficients \( b \) converge to \( e_0 \), and the denominator polynomial \( q \) converges to one, and the error committed by multiplying by the denominator vanishes. Moreover, as \( q \to 1 \), we recover a pole-residue expansion of \( r \) with poles \( \lambda^{(\ell)} \) and residues \( a \). To extend this algorithm for numerators of degree \( m > n - 1 \), it is sufficient to append columns to \( \Phi \). The complete algorithm is given in Algorithm 2.3.

Although the iterates of this algorithm are substantially better conditioned than those of the SK iteration, as illustrated in Figure 2.2, this algorithm is not without its concerns. There are examples of input data where all fixed points are repelling, causing the algorithm to iterate indefinitely [17], which Lefteriu and Antoulas suggest fixing by adding a Newton step. However, this does not address a more subtle issue: although the fixed points of this algorithm often provide excellent rational approximations, as evidenced by Figure 2.2, these fixed points do not satisfy the first
order necessary conditions for the least squares rational approximation problem (1.4). Instead, even when initialized at the least squares optimizer, the gradient associated with the fixed point of both algorithms was substantially larger than that generated using optimization, as illustrated in Figure 2.3. This does not appear to be a numerical artifact because when initialized at the least squares optimizer, the first step changed b by at least $10^{-3}$ in both the SK iteration and Vector Fitting for every n test. This also helps motivate our development of nonlinear least squares approaches in the next two sections.

3. Optimization Using a Polynomial Basis. An alternative to both Loewner framework and the fixed point iterations presented previously is to consider the rational approximation problem in the light of standard optimization algorithms for least squares problems [13]. In this section we will discuss how to apply these results when the rational approximant is parameterized as a ratio of polynomials

$$r(z; a, b) := \frac{p(z; a)}{q(z; b)} = \frac{\sum_{k=0}^{m} a_k \phi_k(z)}{\sum_{k=0}^{n} b_k \psi_k(z)}$$

where $\{\phi_k\}_{k=0}^{m}$ and $\{\psi_k\}_{k=0}^{n}$ are two polynomial bases. This approach has the advantage of being able to represent any degree rational approximant, whereas the pole-residue parameterization described in the next section is restricted to degree $(m, n)$ where $m \geq n - 1$. Unfortunately as with the SK-iteration, the use of a polynomial basis makes this method ill-conditioned and of limited utility for rational approximations of moderate dimension, e.g., $n \approx 20$. However, the ideas developed in this approach are later applied in the next section to construct a real rational approximation. In this section, we first derive how to use Variable Projection (VARPRO) [10] to construct an optimization problem over b alone and then discuss how to construct a real rational approximation.

3.1. Variable Projection. To apply Variable Projection to this rational approximation problem, we first state the optimization problem in terms of two Van-
dermonde matrices $\Phi \in \mathbb{C}^{N \times (m+1)}$ and $\Psi \in \mathbb{C}^{N \times (n+1)}$:

$$
\Phi = \begin{bmatrix}
\phi_0(z_1) & \cdots & \phi_m(z_1) \\
\vdots & \ddots & \vdots \\
\phi_0(z_M) & \cdots & \phi_m(z_M)
\end{bmatrix}, \quad
\Psi = \begin{bmatrix}
\psi_0(z_1) & \cdots & \psi_m(z_1) \\
\vdots & \ddots & \vdots \\
\psi_0(z_M) & \cdots & \psi_m(z_M)
\end{bmatrix},
$$

as then the rational approximation is

$$
\text{minimize}_{a \in \mathbb{C}^{m+1}, b \in \mathbb{C}^{n+1}} \| W[f - \text{diag}(\Psi b)^{-1} \Phi a] \|_2.
$$

The key insight in Variable Projection is that if the nonlinear parameter $b$ is held fixed, $a$ can be written in terms of the pseudoinverse, denoted $+$:

$$
a = [W \text{diag}(\Psi b)^{-1} \Phi]^+ W f.
$$

If we substitute this value of $a$ into (3.3), we recover an equivalent optimization problem over $b$ alone:

$$
\text{minimize}_{b \in \mathbb{C}^{n+1}} \| P_{\Omega(b)}^\perp W f \|_2, \quad \Omega(b) := W \text{diag}(\Psi b)^{-1} \Phi,
$$

and where $P_{\Omega(b)}^\perp$ is the projector onto the orthogonal complement of the range of $\Omega(b)$. Defining the interior of this minimization problem as the residual $r : \mathbb{C}^{n+1} \to \mathbb{C}^N$, we have

$$
r(b) := P_{\Omega(b)}^\perp W f.
$$

Golub and Pereyra then give a formula the Jacobian of $r(b)$ where

$$
\frac{\partial r(b)}{\partial b_k} = -P_{\Omega(b)}^\perp \frac{\partial \Omega(b)}{\partial b_k} \Omega(b)^+ W f - \Omega(b)^+ \frac{\partial \Omega(b)^*}{\partial b_k} P_{\Omega(b)}^\perp W f
$$

where we have invoked Wirtinger calculus [21, App. 2] to extend this result. However, we must be careful here as $r(b)$ is not an analytic function of $b$. Instead we will define the Jacobian of $r(b)$ split into real and imaginary parts:

$$
g(b) := \begin{bmatrix}
\text{Re } r(b) \\
\text{Im } r(b)
\end{bmatrix}
$$

and construct the Jacobian with respect to $b$ also split into real and imaginary parts:

$$
J(b) := \begin{bmatrix}
\frac{\partial \text{Re } r(b)}{\partial b} & \frac{\partial \text{Im } r(b)}{\partial b} \\
\frac{\partial \text{Re } r(b)}{\partial b} & \frac{\partial \text{Im } r(b)}{\partial b}
\end{bmatrix}.
$$

If we define matrices $K(b)$ and $L(b)$ related the two terms in the Jacobian (3.7)

$$
[K(b)]_{:.k} := -P_{\Omega(b)}^\perp \frac{\partial \Omega(b)}{\partial \text{Re } b_k} \Omega(b)^+ W f, \quad [L(b)]_{:.k} := -\Omega(b)^+ \frac{\partial \Omega(b)^*}{\partial \text{Re } b_k} P_{\Omega(b)}^\perp W f,
$$

where the derivative of $\Omega(b)$ is

$$
\frac{\partial \Omega(b)}{\partial \text{Re } b_k} = -W \text{diag}(\Psi b)^{-1} \frac{\partial \text{diag}(\Psi b)}{\partial \text{Re } b_k} \text{diag}(\Psi b)^{-1} \Phi
$$

and

$$
= -W \text{diag}(\Psi e_k) \text{diag}(\Psi b)^{-2} \Phi.
$$
Algorithm 3.1 Residual and Jacobian for Complex Polynomial Parameterization

\begin{verbatim}
Input : Polynomial coefficients b ∈ C^{n+1}
Output : Residual r ∈ R^{2N} and Jacobian J ∈ R^{(2N)×(2n+2)}
1 Form Ω from (3.5): Ω ← W diag(Ψb)^{-1}Ψ;
2 Compute short form QR decomposition: QR ← Ω;
3 r ← WF - QQ^*WF;
4 r ← Re r;
5 a ← R^*Q^*WF;
6 [K]_{k} ← [I - QQ^*]W diag(Ψe_k) diag(Ψb)^{-2}Φa \quad k = 0, \ldots, n;
7 [L]_{k} ← QR^*Ψ^* diag(Ψe_k)^* diag(Ψb)^{-2*}W^*r \quad k = 0, \ldots, n;
8 J ←
\begin{bmatrix}
    Re K + Re L & - Im K + Im L \\
    Im K + Im L & Re K - Re L
\end{bmatrix};
\end{verbatim}

Using these two matrices we note that by the chain rule, derivatives with respect to Im b_k simply multiply K(b) and L(b) by i. Hence the Jacobian J(b) is

\begin{equation}
J(b) = \begin{bmatrix}
    Re K(b) + Re L(b) & - Im K(b) + Im L(b) \\
    Im K(b) + Im L(b) & Re K(b) - Re L(b)
\end{bmatrix},
\end{equation}

recalling that the part of the Jacobian corresponding to L appears with a derivative with respect to \( b_k \). An algorithm to construct this residual and Jacobian is given in Algorithm 3.1.

3.2. Real Rational Approximation. If we wish to impose the constraint the approximant \( r \) is a real rational function, \( r \in \mathbb{R}_{m,n}(\mathbb{R}) \), one approach is modify the parameterization such that \( r \) is necessarily in this class. Using the polynomial basis, we can enforce this constraint by choosing the bases \( \{ϕ_k\}_{k=0}^m \) and \( \{ψ_k\}_{k=0}^n \) consist solely of real polynomials (polynomials with only real coefficients), and then requiring the coefficients \( a \) and \( b \) to both be real. This causes several changes to our formula for the Jacobian. First, as \( b \) is real, the Jacobian now only has \( n+1 \) columns. Next, we need to ensure that the solution for \( a \) is real as well as when the projector \( P_{θ(\Omega)} \) is used. To do so, we instead use the projector from \( Ω(b) \) split into real and imaginary parts \( P_{θ(\Omega)} \):

\begin{equation}
Ω(b) := \begin{bmatrix}
    Re Ω(b) \\
    Im Ω(b)
\end{bmatrix}.
\end{equation}

Then we form the Jacobian using this projector as before, but instead using \( WF \) split into real and imaginary parts:

\begin{equation}
[J(b)]_{k} = -P_{Ω(b)}^+ \frac{∂Ω(b)}{∂ Re b_k} Ω(b)^+ f - Ω(b)^+ \frac{∂Ω(b)}{∂ Im b_k} P_{Ω(b)}^+ f; \quad f = \begin{bmatrix}
    Re WF \\
    Im WF
\end{bmatrix}.
\end{equation}

These modifications are summarized in Algorithm 3.2.

3.3. Normalization and Conditioning. As with the SK-iteration, we now face a choice of how to remove the additional degree of freedom in our choice of \( b \). One simple option would be to simply fix one of the entries; for example, forcing \( b_n = 1 \) which then yields small Jacobian with only \( 2n \) columns. Another option is to constrain the norm of \( b \), e.g., \( ||b||_2 = 1 \), which is more numerically sound if the
Algorithm 3.2 Residual and Jacobian for Real Polynomial Parameterization

\[\text{Input : } \text{Polynomial coefficients } b \in \mathbb{R}^{n+1} \]
\[\text{Output : } \text{Residual } r \in \mathbb{R}^N \text{ and Jacobian } J \in \mathbb{R}^{(2N) \times (n+1)} \]

1. Form \( \Omega \) from (3.5): \( \Omega \leftarrow W \operatorname{diag}(\Psi b)^{-1} \Phi \);

2. \( \Omega \leftarrow \begin{bmatrix} \operatorname{Re} \Omega \\ \operatorname{Im} \Omega \end{bmatrix} \)
\( f \leftarrow \begin{bmatrix} \operatorname{Re} W f \\ \operatorname{Im} W f \end{bmatrix} ; \)

3. Compute short form QR decomposition: \( QR \leftarrow \Omega ; \)

4. \( r \leftarrow f - Q^T f \quad r \leftarrow [r]_{1.5} + i[r]_{N+1.2} ; \)

5. \( a \leftarrow R^T Q f \)

6. \( \begin{bmatrix} K' \\ L' \end{bmatrix} \leftarrow \begin{bmatrix} I - Q Q^T \end{bmatrix} \begin{bmatrix} \operatorname{Re} \operatorname{diag}(\Psi e_k) \operatorname{diag}(\Psi b)^{-2} \Phi a \\ \operatorname{Im} \operatorname{diag}(\Psi e_k) \operatorname{diag}(\Psi b)^{-2} \Phi a \end{bmatrix} \quad k = 0, \ldots, n ; \)

7. \( \begin{bmatrix} K' \\ L' \end{bmatrix} \leftarrow \begin{bmatrix} \operatorname{Re} \Phi^* \operatorname{diag}(\Psi e_k)^* \operatorname{diag}(\Psi b)^{-2} W r^* \\ \operatorname{Im} \Phi^* \operatorname{diag}(\Psi e_k)^* \operatorname{diag}(\Psi b)^{-2} W r^* \end{bmatrix} \quad k = 0, \ldots, n ; \)

8. \( J \leftarrow K + L ; \)

**Fig. 3.1.** Here we show two sets of condition numbers relevant to optimization in both the polynomial and pole-residue bases. The left plot shows the condition number associated with finding the linear parameters. For the polynomial basis, this is the condition number of \( \Omega p b q \) denoted by \( \ominus \); for the pole-residue basis, this is the condition number of \( \Lambda p \lambda q \) given in (4.4) denoted by \( \Phi \); for the quadratic partial fraction expansion used in subsection 4.2 this is \( \Theta p b q \) given by (4.11) denoted by \( \Theta \). The right plot shows the condition number of the Jacobian with the polynomial basis using a monic constraint shown as \( \ominus \), and norm constraint shown as \( \Phi \) the condition number of the pole-residue Jacobian is shown as \( \Phi \) for the complex case and \( \Phi \) for the real case. In each case these matrices are evaluated at a local optimum of the CD player model described in Figure 1.1.

Coefficient we fixed is small or zero at the optimum. However, fixing the norm of \( b \) is substantially more difficult to implement; for example one approach would be perform optimization on the Grassmann manifold [7]. Unfortunately, neither approach is ultimately helpful. As shown in Figure 3.1, the condition number of \( \Omega b \) grows rapidly with increasing degree. Similarly, the Jacobian is increasingly ill-conditioned until the loss of precision in the pseudoinverse of \( \Omega b \) causes the condition number to artificially decrease; using the full Jacobian, ignoring its two dimensional nullspace, does not fix the conditioning issues either. This motivates using the pole-residue basis we discuss in the next section.

4. Optimization Using a Partial Fraction Parameterization. An alternative to the ratio of two polynomials used in the previous section is to instead consider the partial fraction expansion of \( r \) into a sum of degree \((0,1)\) rational functions. For a degree \((m,n)\) rational function where \(m \geq n-1\) and \(q\) has \(n\) distinct roots \(\{\lambda_k\}_{k=1}^n\)
we can write
\begin{equation}
   r(z; \mathbf{a}, \mathbf{b}) := \frac{p(z; \mathbf{a})}{q(z; \mathbf{b})} = \frac{\sum_{k=0}^{m} a_k \phi_k(z)}{\sum_{k=0}^{m} b_k \varphi_k(z)} = \sum_{k=1}^{n} \frac{\rho_k}{z - \lambda_k} + \sum_{k=0}^{m-n} c_k \varphi_k(z) =: r(z; \lambda, \rho, c)
\end{equation}

where \( \{\varphi_k\}_{k=0}^{m-n} \) is a basis for polynomials of degree \( m - n \). This partial fraction expansion, also known as a pole-residue expansion, is much better conditioned than the polynomial basis for rational approximation considered in the previous section, as evidenced by Figure 3.1, leading to better optimizers of the least squares rational approximation problem. There is a small price we have paid for this: the pole-residue basis cannot express higher order poles \((z - \lambda)^2, (z - \lambda)^3, \text{etc.}\) However, for any polynomial \( q \) with multiple roots there is another polynomial \( \tilde{q} \) arbitrarily close with distinct roots. Hence for the purposes of rational approximation, even if \( f \) has higher order poles, we can approximate it arbitrarily well in the pole-residue parameterization.

In the following subsections, we first derive the VARPRO residual and Jacobian for this problem and then show how enforce that \( r \) is a real rational function. Here we are forced to modify our parameterization, choosing a partial fraction expansion into a sum of degree (1, 2) rational functions and we reuse portions of the derivation from subsection 3.2.

### 4.1. Variable Projection

To begin, we first write the least squares rational approximation problem using this parameterization in terms of a Cauchy matrix \( C(\lambda) \in \mathbb{C}^{n \times n} \) and a Vandermonde matrix \( \Phi \in \mathbb{C}^{N \times (m-n)} \):

\begin{equation}
   \minimize_{\lambda \in \mathbb{C}^n, \rho \in \mathbb{C}^n, \mathbf{c} \in \mathbb{C}^{m-n}} \|W[f - C(\lambda)\rho - \Phi\mathbf{c}]\|_2.
\end{equation}

where

\begin{equation}
   C(\lambda) := \begin{bmatrix}
   (z_1 - \lambda_1)^{-1} & \cdots & (z_1 - \lambda_n)^{-1} \\
   \vdots & \ddots & \vdots \\
   (z_N - \lambda_1)^{-1} & \cdots & (z_N - \lambda_n)^{-1}
   \end{bmatrix}, \quad \Phi := \begin{bmatrix}
   \varphi_0(z_1) & \cdots & \varphi_m(z_1) \\
   \vdots & \ddots & \vdots \\
   \varphi_0(z_M) & \cdots & \varphi_m(z_M)
   \end{bmatrix}.
\end{equation}

As with optimization in the polynomial basis, it is helpful to define a single matrix function \( \Lambda(\lambda) \), analogous to \( \Omega(\mathbf{b}) \) in (3.5):

\begin{equation}
   \Lambda(\lambda) := \begin{bmatrix}
   WC(\lambda) & \Phi
   \end{bmatrix},
\end{equation}

leaving the optimization problem:

\begin{equation}
   \minimize_{\lambda \in \mathbb{C}^n, \mathbf{d} \in \mathbb{C}^m} \|Wf - \Lambda(\lambda)\mathbf{d}\|_2, \quad \mathbf{d} = \begin{bmatrix}
   \rho \\
   \mathbf{c}
   \end{bmatrix}.
\end{equation}

Then, as before, we use VARPRO to convert this into an optimization problem over \( \lambda \) alone:

\begin{equation}
   \minimize_{\lambda \in \mathbb{C}^n} \|P^\perp_{\Lambda(\lambda)}Wf\|_2 \quad \text{with residual} \quad r(\lambda) := P^\perp_{\Lambda(\lambda)}Wf.
\end{equation}

Then, defining the two terms in the VARPRO Jacobian \( \mathbf{K} \) and \( \mathbf{L} \) analogously to (3.10),

\begin{equation}
   \left[ \mathbf{K}(\lambda) \right]_{i,k} := -P^\perp_{\Lambda(\lambda)} \frac{\partial \Lambda(\lambda)}{\partial \text{Re} \lambda_k} \Lambda(\lambda)^*Wf, \quad \left[ \mathbf{L}(\lambda) \right]_{i,k} := -\Lambda(\lambda)^* \frac{\partial \Lambda(\lambda)^*}{\partial \text{Re} \lambda_k} P^\perp_{\Lambda(\lambda)}Wf,
\end{equation}
Algorithm 4.1 Residual and Jacobian for Partial Fraction Parameterization

Input : Poles $\lambda \in \mathbb{C}^n$

Output : Residual $\mathbf{r} \in \mathbb{R}^{2N}$ and Jacobian $\mathbf{J} \in \mathbb{R}^{(2N)\times(2n)}$

1 Form $\mathbf{A} \leftarrow \Lambda(\lambda)$ using (4.4);
2 Compute the short form QR decomposition $\mathbf{Q}\mathbf{R} \leftarrow \Lambda$;
3 Compute residual $\mathbf{r} \leftarrow \mathbf{WF} - \mathbf{Q}\mathbf{Q}^* \mathbf{WF}$;

4 $\mathbf{z} \leftarrow \begin{bmatrix} \text{Re}\mathbf{r} \\ \text{Im}\mathbf{r} \end{bmatrix}$
5 $\begin{bmatrix} \rho \\ \mathbf{c} \end{bmatrix} \leftarrow \mathbf{R}^* \mathbf{Q}^* \mathbf{WF}$;
6 Build $[\Lambda^*]_{j,k} = -(z_j - \lambda_k)^{-2}$;
7 $\mathbf{K} \leftarrow -[\mathbf{I} - \mathbf{Q}\mathbf{Q}^*] \mathbf{W} \Lambda^* \text{diag}(\rho)$;
8 $\mathbf{L} \leftarrow -\mathbf{Q} \mathbf{R}^* \text{diag}(\Lambda^* \mathbf{r})$;
9 $\mathbf{J} \leftarrow \begin{bmatrix} \text{Re}\mathbf{K} + \text{Re}\mathbf{L} & -\text{Im}\mathbf{K} + \text{Im}\mathbf{L} \\ \text{Im}\mathbf{K} + \text{Im}\mathbf{L} & \text{Re}\mathbf{K} - \text{Re}\mathbf{L} \end{bmatrix}$;

where the derivative $\Lambda(\lambda)$ with respect to $\lambda_k$ is

$$
\frac{\partial \Lambda(\lambda)}{\partial \text{Re}\lambda_k} = -\begin{bmatrix} (z_1 - \lambda_k)^{-2} \\ \vdots \\ (z_N - \lambda_k)^{-2} \end{bmatrix} \mathbf{e}_k^\top,
$$

where $\mathbf{e}_k$ is the $k$th unit vector. Then, using this $\mathbf{K}(\lambda)$ and $\mathbf{L}(\lambda)$ we can build the the Jacobian using (3.13) as before. In building the residual and Jacobian in Algorithm 4.1, we also exploit the rank-1 structure of $\partial \Lambda(\lambda)/\partial \text{Re}\lambda_k$, to build $\mathbf{K}$ and $\mathbf{L}$ using matrix-matrix products rather than a loop over $k$ as in Algorithm 3.1.

4.2. Real Rational Approximation. It is not simple to construct a real rational approximation in a pole-residue basis. As with the polynomial basis, we can require the basis for the polynomial component $\{\varphi_k\}_{k=0}^m$ consist of real polynomials and that the coefficients $\mathbf{c}$ be real. However, more complicated constraints are required for the pole-residue portion to ensure that $r(\overline{z}) = \overline{r(z)}$. Namely, for every $\lambda_k$ with nonzero imaginary part that there is another pole $\overline{\lambda}_k$ that is its complex conjugate pair, $\lambda_k = \overline{\lambda}_k$ and that this same relationship applies to the residues, $\rho_k = \overline{\rho}_k$. Naively enforcing these constraints is not simple: these pairings can appear if poles leave the real line and disappear if poles enter the real line. Alternatively, we could automatically include the conjugate of every non-real $\lambda_k$ but the degree of the rational approximation will change whenever a $\lambda_k$ becomes real. If we instead try to work with an implicit parameterization of the poles, such as parametrizing a pair of poles as roots of quadratic polynomial $q(z) = z^2 + b_1z + b_0$ this parameterization is not differentiable when $q$ has a multiple root. Instead, here we develop an approach based on a partial fraction expansion of $r$ into a sum of $(1, 2)$ rational functions plus the remaining $m - n$ polynomial terms:

$$
(4.9) \quad r(z; \mathbf{a}, \mathbf{b}, \mathbf{c}) = \sum_{k=0}^{m-n} c_k \varphi_k(z) + \begin{cases} 
\sum_{k=1}^{[n/2]} \frac{a_{2k} z + a_{2k-1}}{z^2 + b_{2k} z + b_{2k-1}}, & n \text{ even;} \\
\frac{a_n}{z + b_n} + \sum_{k=1}^{[n/2]} \frac{a_{2k} z + a_{2k-1}}{z^2 + b_{2k} z + b_{2k-1}}, & n \text{ odd;}
\end{cases}
$$
where \( \mathbf{a}, \mathbf{b} \in \mathbb{R}^n \text{ and } \mathbf{c} \in \mathbb{R}^{n-n} \). This is a middle ground between the pole-residue approach we used before and the polynomial basis considered in section 3 that is better conditioned yet still allows us to easily enforce that \( r \) is a real rational function by requiring \( \mathbf{a}, \mathbf{b}, \text{ and } \mathbf{c} \) to be real.

The derivation of the residual and Jacobian for this parameterization largely follows that of subsection 3.2. Defining \( \Theta(\mathbf{b}) \) in an analogous role to \( \Omega(\mathbf{b}) \) and \( \Lambda(\lambda) \), we state the optimization problem as

\[
\text{(4.10)} \quad \min_{\mathbf{a}, \mathbf{b} \in \mathbb{R}^n, \mathbf{c} \in \mathbb{R}^{n-n}} \left\| \begin{bmatrix} \text{Re } \mathbf{Wf} \\ \text{Im } \mathbf{Wf} \end{bmatrix} - \begin{bmatrix} \text{Re } \Theta(\mathbf{b}) \\ \text{Im } \Theta(\mathbf{b}) \end{bmatrix} \begin{bmatrix} \mathbf{a} \\ \mathbf{c} \end{bmatrix} \right\|_2,
\]

where

\[
\text{(4.11)} \quad \Theta(\mathbf{b}) := \begin{cases} 
\mathbf{W} \left[ \hat{\hat{\Omega}}_1([\mathbf{b}]_{1:2}) \cdots \hat{\hat{\Omega}}([\mathbf{b}]_{n-1,n}) \right] \Phi, & \text{if } n \text{ is even;} \\
\mathbf{W} \left[ \hat{\hat{\Omega}}_1([\mathbf{b}]_{1:2}) \cdots \hat{\hat{\Omega}}([\mathbf{b}]_{n-2,n-1}) \right] (\mathbf{z} + \mathbf{b}_n)^{-1} \Phi, & \text{if } n \text{ is odd;}
\end{cases}
\]

and where \( \hat{\hat{\Omega}}(\mathbf{b}) \) defined analogously to \( \Omega(\mathbf{b}) \) for a degree \((1,2)\) rational function in the monomial basis with a monic constraint:

\[
\text{(4.12)} \quad \hat{\hat{\Omega}}(\mathbf{b}) := \text{diag} \left( \begin{bmatrix} z_1^2 + b_2 z_1 + b_1 \\ \\ \\
\end{bmatrix} \right)^{-1} \begin{bmatrix} z_1 & 1 \\
\vdots & \vdots \\
z_N & z_N \\
\end{bmatrix}
\]

and \( \Phi \) is defined as in (4.3). Then, after applying VARPRO, our residual is

\[
\text{(4.13)} \quad \mathbf{g}(\mathbf{b}) = P^\perp_{\hat{\hat{\Theta}}}(\mathbf{b}) \mathbf{f}, \quad \hat{\hat{\Omega}}(\mathbf{b}) = \begin{bmatrix} \text{Re } \Theta(\mathbf{b}) \\ \text{Im } \Theta(\mathbf{b}) \end{bmatrix} \mathbf{f} = \begin{bmatrix} \text{Re } \mathbf{Wf} \\ \text{Im } \mathbf{Wf} \end{bmatrix}.
\]

Then, computing the Jacobian is similar to subsection 3.2, except now the Jacobian is split into two column blocks, with an additional one column block if \( n \) is odd. This formula is given in Algorithm 4.2. Then once we have found an optimum \( \mathbf{b} \), we can easily convert back to a pole-residue form, using the quadratic formula to compute the roots of each term and then compute their corresponding residues.

Although this approach has used elements of the polynomial basis to enforce the real constraint, the optimization problem has not become substantially more ill-conditioned than the pole-residue approach of the previous section. As illustrated in Figure 3.1, the condition number of this approach stays close to that of the pole-residue basis. We suspect that this is due to the fact that this case has used a partial fraction expansion into degree \((1,2)\) rational functions whereas the pole-residue approach can be interpreted as an expansion into \((0,1)\) rational functions.

5. Numerical Examples. As the previous sections have included several examples illustrating the performance of our optimization approach using both polynomial and partial fraction bases for both real and complex rational approximation, here we focus our attention to features not addressed in previous examples. In the first example we show the utility of enforcing the real constraint and in the second we consider a rational approximation problem with a nontrivial weight matrix \( \mathbf{W} \) related to the projected \( \mathcal{H}_2 \) model reduction problem.

5.1. Employing the Real Constraint. As an example of how requiring the real constraint can prove beneficial, Figure 5.1 illustrates the rational fits to only samples with positive imaginary part. Without imposing the real constraint, the resulting approximation only fits where there are samples with positive part. However by adding the constraint that \( r \) be real, the resulting approximation does equally well on both halves of the data.
complex rational
real rational

Construct a real least squares rational approximation of degree

As a step in the model reduction process, it is necessary to

\[ \text{Residual and Jacobian for Real Partial Fraction Parameterization} \]

\[ \text{Input: Parameters for quadratic expansion } b \in \mathbb{R}^n \]
\[ \text{Output: Residual } r \in \mathbb{R}^n \text{ and Jacobian } J \in \mathbb{R}^{(2N) \times n} \]

1. Form \( \Theta \leftarrow \Theta(b) \) from (4.11) and \( \Theta \leftarrow \begin{bmatrix} \text{Re } \Theta \\ \text{Im } \Theta \end{bmatrix} \);
2. Compute the short form QR decomposition \( QR \leftarrow \Theta \);
3. Define \( f \leftarrow \begin{bmatrix} \text{Re } Wf \\ \text{Im } Wf \end{bmatrix} \);
4. Compute residual \( r \leftarrow f - QQ^*f \) \( r \leftarrow [r]_{1:N} + i [r]_{N+1:2N} \);
5. Compute linear coefficients \( \begin{bmatrix} a \\ c \end{bmatrix} \leftarrow d \leftarrow R^*QQ^*f; \)
6. for \( k = 1, \ldots, |n/2| \) do
7. \[ \begin{bmatrix} [K]_{2k-1} \\ [K]_{2k} \end{bmatrix} \leftarrow [I - QQ^*] \begin{bmatrix} \text{Re } W \text{ diag}(z^2 + b_{2k}z + b_{2k-1})^{-2}(a_{2k}z + a_{2k-1}) \\ \text{Im } W \text{ diag}(z^2 + b_{2k}z + b_{2k-1})^{-2}(a_{2k}z + a_{2k-1}) \end{bmatrix}; \]
8. \[ \begin{bmatrix} [L]_{2k-1} \\ [L]_{2k} \end{bmatrix} \leftarrow \begin{bmatrix} \Theta \end{bmatrix} \text{ where } \Theta \text{ is defined in (4.11)} \begin{bmatrix} \text{Re } \Phi^* \text{ diag}(z^2 + b_{2k}z + b_{2k-1})^{-2}W^*r \\ \text{Im } \Phi^* \text{ diag}(z^2 + b_{2k}z + b_{2k-1})^{-2}W^*r \end{bmatrix}; \]
9. if \( n \) is odd then
10. \[ \begin{bmatrix} [K]_{2k-1} \\ [K]_{2k} \end{bmatrix} \leftarrow [I - QQ^*] \begin{bmatrix} \text{Re } W \text{ diag}(z + b_n)^{-2}a_n \\ \text{Im } W \text{ diag}(z + b_n)^{-2}a_n \end{bmatrix}; \]
11. \[ \begin{bmatrix} [L]_{2k-1} \\ [L]_{2k} \end{bmatrix} \leftarrow \text{ where } \Theta \text{ is defined in (4.11)} \begin{bmatrix} \text{Re } \Phi^* \text{ diag}(z + b_n)^{-2}W^*r \\ \text{Im } \Phi^* \text{ diag}(z + b_n)^{-2}W^*r \end{bmatrix}; \]
12. \[ J \leftarrow K + L. \]

**Algorithm 4.2** Residual and Jacobian for Real Partial Fraction Parameterization

**Fig. 5.1.** The samples of the CD player model described in Figure 1.1 along with degree (5, 6) rational fits using a partial fraction expansion with and without the real constraint when fitting to samples with \( \text{Im } z > 0 \).

**5.2. Application to Projected \( \mathcal{H}_2 \) Model Reduction.** In recent work by the authors, the \( \mathcal{H}_2 \) norm is approximated by its projection onto a finite dimensional subspace [15]. Then, as a step in the model reduction process, it is necessary to construct a real least squares rational approximation of degree \((n - 1, n)\) in a weighted
FIG. 5.2. The residual norm on the weighted rational fitting problem emerging from the projected $H_2$ approach as described in subsection 5.2 using the real partial fraction expansion described in subsection 4.2 and the vectfit3 implementation of vector fitting which does not support non-diagonal weightings.

norm:

$$\minimize_{r \in \mathcal{R}_{n-1,n}(\mathbb{R})} \| W[f(Z) - r(Z)] \|_2$$

where the weight matrix $W$ is the inverse square root of a Cauchy matrix $M(z)$:

$$W = M(z)^{-1/2}, \quad M(z) = \begin{bmatrix} (z_1 + \bar{z}_1)^{-1} & \cdots & (z_1 + \bar{z}_N)^{-1} \\ \vdots & \ddots & \vdots \\ (z_N + \bar{z}_1)^{-1} & \cdots & (z_N + \bar{z}_N)^{-1} \end{bmatrix}$$

and each $z_j$ is in the right half plane. Using Demmel’s results [5], we can compute the SVD of $M(z) = U\Sigma V^*$ to high relative accuracy and set $W = \Sigma^{-1/2}U^*$.

As an example of this weighted problem, Figure 5.2 considers the CD player model sampled a sequence of points with imaginary part uniformly sampled between $-1000i$ and $1000i$: 80 points with $\text{Re} z = 0.001$, 40 points with $\text{Re} z = 0.01$, 20 points with $\text{Re} z = 0.1$, and 10 points with $\text{Re} z = 1$. As expected, the vectfit3 implementation of vector fitting does worse in almost every case as it does not support non-diagonal weight matrices.

6. Discussion. Here we have shown how to construct least squares rational approximants using standard optimization techniques in two bases, a ratio of polynomials and a more stable partial fraction expansion, and with and without constraining the rational approximant to be real. Although this optimization approach often finds spurious local minima, we have found that the AAA algorithm provides an effective initialization. Moreover, unlike existing approaches, we are able to find rational approximants that satisfy the first order necessary conditions to high precision.

Our focus has been on the scalar rational approximation problem, however many applications in systems theory seek a rational function with vector or matrix valued output:

$$\mathcal{R}_{m,n}(\mathbb{C}, \mathbb{C}^{s \times t}) := \{ q(z)^{-1} P(z) | q \in \mathcal{P}_n(\mathbb{C}), \ P \in \mathcal{P}_m(\mathbb{C}, \mathbb{C}^{s \times t}) \}$$
where \( \mathcal{P}_m(\mathbb{C}, \mathbb{C}^{n \times t}) \) is the space of matrix polynomials of degree \( m \). If we then seek to perform a matrix-valued rational approximation using the Frobenius norm

\[
\text{minimize}_{R \in \mathcal{P}_{m,n}(\mathbb{C}, \mathbb{C}^{s \times t})} \sum_{j=1}^{N} \| R(z_j) - F(z_j) \|_F
\]

we can easily generalize our approaches to this problem. For example, considering a pole-residue expansion of a degree \((n - 1, n)\) rational function, \( R(z) \),

\[
R(z) = \sum_{k=1}^{n} \frac{\rho_k}{z - \lambda_k}, \quad R : \mathbb{C} \to \mathbb{C}^{s \times t}, \rho_k \in \mathbb{C}^{s \times t}.
\]

we can similarly use VARPRO to implicitly solve for linear parameters \( \rho_k \). However, in the context of model reduction, it is often desired to impose a constraint that each \( \rho_k \) is rank-1, so that the dimension of the reduced order model is \( n \). It is an open question as to how best to incorporate this constraint.

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