Adv Comput Math (2017) 43:151–170
DOI 10.1007/s10444-016-9481-0

Minimal polynomial and reduced rank extrapolation methods are related

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Received: 6 April 2016 / Accepted: 9 August 2016 /
Published online: 14 September 2016
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Abstract Minimal Polynomial Extrapolation (MPE) and Reduced Rank Extrapolation (RRE) are two polynomial methods used for accelerating the convergence of sequences of vectors $\{\boldsymbol{x}_m\}$. They are applied successfully in conjunction with fixed-point iterative schemes in the solution of large and sparse systems of linear and nonlinear equations in different disciplines of science and engineering. Both methods produce approximations $\boldsymbol{s}_k$ to the limit or antilimit of $\{\boldsymbol{x}_m\}$ that are of the form $\boldsymbol{s}_k = \sum_{i=0}^{k} \gamma_i \boldsymbol{x}_i$ with $\sum_{i=0}^{k} \gamma_i = 1$, for some scalars γ_i. The way the two methods are derived suggests that they might, somehow, be related to each other; this has not been explored so far, however. In this work, we tackle this issue and show that the vectors $\boldsymbol{s}_k^{\text{MPE}}$ and $\boldsymbol{s}_k^{\text{RRE}}$ produced by the two methods are related in more than one way, and independently of the way the $\boldsymbol{x}_m$ are generated. One of our results states that RRE stagnates, in the sense that $\boldsymbol{s}_k^{\text{RRE}} = \boldsymbol{s}_{k-1}^{\text{RRE}}$, if and only if $\boldsymbol{s}_k^{\text{MPE}}$ does not exist. Another result states that, when $\boldsymbol{s}_k^{\text{MPE}}$ exists, there holds

$$\mu_k \boldsymbol{s}_k^{\text{RRE}} = \mu_{k-1} \boldsymbol{s}_{k-1}^{\text{RRE}} + \nu_k \boldsymbol{s}_k^{\text{MPE}} \quad \text{with} \quad \mu_k = \mu_{k-1} + \nu_k,$$

for some positive scalars μ_k, μ_{k-1}, and ν_k that depend only on $\boldsymbol{s}_k^{\text{RRE}}$, $\boldsymbol{s}_{k-1}^{\text{RRE}}$, and $\boldsymbol{s}_k^{\text{MPE}}$, respectively. Our results are valid when MPE and RRE are defined in any weighted inner product and the norm induced by it. They also contain as special cases the known results pertaining to the connection between the method of Arnoldi and the method of generalized minimal residuals, two important Krylov subspace methods for solving nonsingular linear systems.

Communicated by: Raymond H. Chan

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Keywords Vector extrapolation methods · Minimal polynomial extrapolation (MPE) · Reduced rank extrapolation (RRE) · Krylov subspace methods · Method of Arnoldi · Method of generalized minimal residuals · GMRES

Mathematics Subject Classification (2010) 65B05 · 65F10 · 65F50 · 65H10

1 Introduction

Minimal Polynomial Extrapolation (MPE) of Cabay and Jackson [5] and *Reduced Rank Extrapolation* (RRE) of Kaniel and Stein [18], Eddy [7], and Mešina [19] are two polynomial methods of convergence acceleration for sequences of vectors.[1] They have been used successfully in different areas of science and engineering in accelerating the convergence of sequences that arise, for example, from application of fixed-point iterative schemes to large and sparse linear or nonlinear systems of equations.

These methods and others were reviewed by Smith, Ford, and Sidi [32], Sidi, Ford, and Smith [29] and, more recently, by Sidi [27]. Their convergence and stability properties were analyzed in the papers by Sidi [23, 26], Sidi and Bridger [28], and Sidi and Shapira [30, 31]. Their connection with known Krylov subspace methods for the solution of linear systems of equations was explored in Sidi [24]. In Ford and Sidi [11], they were shown to satisfy certain interesting recursion relations. Efficient algorithms for their implementation that are stable numerically and economical computationally and storagewise were designed in Sidi [25]. Finally, Chapter 4 of the book by Brezinski and Redivo Zaglia [3] is devoted completely to vector extrapolation methods and their various properties.

From the way they are derived, one might suspect that MPE and RRE are somehow related. Despite being intriguing and of interest in itself, this subject has not been investigated until now, however. In this work, we undertake precisely this investigation and show that the two methods are indeed very closely related in more than one way. A partial description of the results of this investigation are given in the next paragraph.

Let $\{\boldsymbol{x}_m\}$ be an *arbitrary* sequence of vectors in $\mathbb{C}^N$ endowed with a general *weighted* (not necessarily standard Euclidean) inner product and the norm induced by it, and let $\boldsymbol{s}_k^{\text{MPE}}$ and $\boldsymbol{s}_k^{\text{RRE}}$ be the vectors (approximations to $\lim_{m\to\infty}\boldsymbol{x}_m$ when this limit exists, for example) produced by MPE and RRE from the $k+2$ vectors $\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_{k+1}$. It is known that $\boldsymbol{s}_k^{\text{RRE}}$ always exists, but $\boldsymbol{s}_k^{\text{MPE}}$ may not always exist. One of our results states that, RRE stagnates, in the sense that

$$\boldsymbol{s}_k^{\text{RRE}} = \boldsymbol{s}_{k-1}^{\text{RRE}} \quad \Leftrightarrow \quad \boldsymbol{s}_k^{\text{MPE}} \text{ does not exist.} \tag{1.1}$$

[1] The formulations of RRE given in Kaniel and Stein [18] and Mešina [19] are essentially the same, but they are entirely different from that in Eddy [7]. The mathematical equivalence of the different formulations is shown in Smith, Ford, and Sidi in [32].

Another result states that, when $\boldsymbol{s}_k^{\scriptscriptstyle MPE}$ exists, there holds

$$\mu_k \boldsymbol{s}_k^{\scriptscriptstyle RRE} = \mu_{k-1}\boldsymbol{s}_{k-1}^{\scriptscriptstyle RRE} + \nu_k \boldsymbol{s}_k^{\scriptscriptstyle MPE} \quad \text{with} \quad \mu_k = \mu_{k-1} + \nu_k, \tag{1.2}$$

for some positive scalars μ_k, μ_{k-1}, and ν_k that depend only on $\boldsymbol{s}_k^{\scriptscriptstyle RRE}$, $\boldsymbol{s}_{k-1}^{\scriptscriptstyle RRE}$, and $\boldsymbol{s}_k^{\scriptscriptstyle MPE}$, respectively. The precise results and the conditions under which they hold will be given in the next sections.[2]

When the sequence $\{\boldsymbol{x}_m\}$ is generated from a *linear* nonsingular system of equations $\boldsymbol{x} = \boldsymbol{T}\boldsymbol{x} + \boldsymbol{d}$ via the fixed-point iterative scheme $\boldsymbol{x}_{m+1} = \boldsymbol{T}\boldsymbol{x}_m + \boldsymbol{d}$, $m = 0, 1, \ldots,$ starting with some initial vector $\boldsymbol{x}_0$, the vectors $\boldsymbol{s}_k^{\scriptscriptstyle MPE}$ and $\boldsymbol{s}_k^{\scriptscriptstyle RRE}$ are precisely those generated by, respectively, the Full Orthogonalization Method (FOM) and the method of Generalized Minimal Residuals (GMR)—two important Krylov subspace methods for solving linear systems—as these are being applied to the linear system $(\boldsymbol{I} - \boldsymbol{T})\boldsymbol{x} = \boldsymbol{d}$, starting with $\boldsymbol{x}_0$ as the initial approximation to the solution. This is so provided all four methods are defined using the same weighted inner product and the norm induced by it.[3]

FOM was developed by Arnoldi [1], who also presented a very elegant algorithm, which employs an interesting process called the *Arnoldi–Gram–Schmidt process*, for computing an orthonormal basis for a Krylov subspace. For a discussion of FOM and more, see also Saad [20]. Different algorithms were given for GMR by Axelsson [2], by Young and Jea [37], by Eisenstat, Elman, and Schultz [9], known as *Generalized Conjugate Residuals* (GCR), and by Saad and Schultz [22], known as GMRES. GMRES also uses the Arnoldi–Gram–Schmidt process, and is known to be the best implementation of GMR. For Krylov subspace methods in general, see the books by Greenbaum [12], Saad [21], and van der Vorst [33]. The methods FOM and GMRES were also formulated in Essai [10] in terms of weighted inner products and norms induced by them; see also Güttel and Pestana [17].

Now, there are interesting connections between the vectors generated by FOM and GMR, and by further Krylov subspace methods, and these connections have been explored in Brown [4] and Weiss [35] originally. This topic has been analyzed further in the papers by Gutknecht [15, 16], Weiss [36], Zhou and Walker [38], Walker [34], Cullum and Greenbaum [6], and Eiermann and Ernst [8], by using weighted inner products and norms induced by them.

In view of the mathematical equivalence of MPE to FOM and of RRE to GMR *when* $\{\boldsymbol{x}_m\}$ *is generated from linear systems*, the results of the present work for MPE and RRE [in particular, (1.1) and (1.2)] are precisely those of [4] and [35] in the presence of such $\{\boldsymbol{x}_m\}$. Clearly, our results pertaining to the relation between MPE and RRE have a larger scope than those pertaining to FOM and RRE because they apply to sequences obtained from nonlinear systems, as well as linear ones, while

[2]Throughout this work, we will use boldface lowercase letters to denote column vectors. In particular, we will denote the zero column vector by $\mathbf{0}$. Similarly, we will use boldface upper case letters to denote matrices.

[3]MPE and RRE were originally defined in $\mathbb{C}^N$ with the standard Euclidean inner product and the norm induced by it. In subsequent work by the author and his co-authors, their definitions were generalized by allowing general inner products and norms. The algorithms for implementing MPE and RRE given in [25] still use the standard Euclidean inner product and the norm induced by it, however.

FOM and RRE apply to linear systems only. Actually, our results apply to *arbitrary* sequences $\{\boldsymbol{x}_m\}$, independently of how these sequences are generated. In this sense, the connection between MPE and RRE can be viewed as being of a *universal* nature. We wish to emphasize that (i) a priori, it cannot be assumed that MPE and RRE are related when applied to vector sequences $\{\boldsymbol{x}_m\}$ arising from nonlinear systems, and (ii) in case there is a relationship, it cannot be concluded, a priori, what form it will assume. In view of this, the fact that MPE and RRE are related as in (1.1) and (1.2) in the presence of *arbitrary* sequences $\{\boldsymbol{x}_m\}$, whether generated linearly or nonlinearly or otherwise, is quite surprising.

The purpose of this work is twofold:

1. In the next section, we (i) redefine MPE and RRE using a weighted inner product and the norm induced by it, and (ii) develop a *unified* algorithm for their implementation, thus also providing the theoretical background necessary for the rest of this work. We note that these developments are completely new and have not been given before. They form an essential part of the proofs of the main results of Section 3. Sometimes, we will refer to the redefined MPE and RRE as *weighted* MPE and RRE.
2. In Section 3, we state and prove our main results showing that MPE and RRE, as redefined in Section 2, are closely related. Following this, in Section 4, we discuss the application of our results to sequences $\{\boldsymbol{x}_m\}$ generated from a linear nonsingular system of equations via fixed-point iterative schemes, and show that our main results reduce to the known analogous results of [4] and [35] that pertain to FOM and GMR, also when all four methods are defined using a weighted inner product and the norm induced by it.

The weighted inner product $\langle\cdot,\cdot\rangle$ and the norm $[\![\cdot]\!]$ induced by it (both in $\mathbb{C}^N$) are defined as in

$$\langle \boldsymbol{y}, \boldsymbol{z}\rangle = \boldsymbol{y}^*\boldsymbol{M}\boldsymbol{z} \quad \text{and} \quad [\![\boldsymbol{z}]\!] = \sqrt{\langle \boldsymbol{z}, \boldsymbol{z}\rangle} = \sqrt{\boldsymbol{z}^*\boldsymbol{M}\boldsymbol{z}}, \tag{1.3}$$

where $\boldsymbol{M} \in \mathbb{C}^{N\times N}$ is a hermitian positive definite matrix.[4] The matrix $\boldsymbol{M}$ is fixed throughout this work.

For the standard l_2 (Euclidean) inner product and the vector norm induced by it, we will use the notation

$$(\boldsymbol{y}, \boldsymbol{z}) = \boldsymbol{y}^*\boldsymbol{z} \quad \text{and} \quad \|\boldsymbol{z}\| = \sqrt{\boldsymbol{z}^*\boldsymbol{z}}. \tag{1.4}$$

A most useful theoretical tool that makes our study of MPE and RRE run smoothly is a generalization of the QR factorization of matrices, which we call the *weighted QR factorization*. This version of the QR factorization seems to have been defined and studied in detail originally in the papers by Gulliksson and Wedin [14] and Gulliksson [13]. It turns out to be the most natural extension of the ordinary QR factorization when orthogonality of two vectors $\boldsymbol{y}, \boldsymbol{z} \in \mathbb{C}^N$ is in the sense $\langle \boldsymbol{y}, \boldsymbol{z}\rangle = 0$.

[4] Recall that the most general inner product in $\mathbb{C}^N$ is the weighted inner product that is of the form $\langle \boldsymbol{y}, \boldsymbol{z}\rangle = \boldsymbol{y}^*\boldsymbol{M}\boldsymbol{z}$, $\boldsymbol{M}$ being a hermitian positive definite matrix. Of course, in the simplest case, $\boldsymbol{M} = \mathrm{diag}(\alpha_1, \ldots, \alpha_N)$ with $\alpha_i > 0\ \forall i$, so that $\langle \boldsymbol{y}, \boldsymbol{z}\rangle = \sum_{i=1}^N \alpha_i \overline{y_i}\, z_i$ and $[\![\boldsymbol{z}]\!] = \sum_{i=1}^N \alpha_i |z_i|^2$. Finally, when $\boldsymbol{M} = \boldsymbol{I}$, we recover the standard Euclidean inner product and the norm induced by it.

For convenience, we state the following theorem concerning the weighted QR factorization:

Theorem 1.1 *Let*

$$\boldsymbol{A} = [\,\boldsymbol{a}_1\,|\,\boldsymbol{a}_2\,|\,\cdots\,|\,\boldsymbol{a}_s\,] \in \mathbb{C}^{m\times s}, \quad m \geq s, \quad rank(\boldsymbol{A}) = s.$$

Let also $\boldsymbol{G} \in \mathbb{C}^{m\times m}$ be hermitian positive definite and define the weighted inner product $\langle\cdot,\cdot\rangle$ via $\langle \boldsymbol{y}, \boldsymbol{z}\rangle = \boldsymbol{y}^*\boldsymbol{G}\boldsymbol{z}$. Then there exist a matrix $\boldsymbol{Q} \in \mathbb{C}^{m\times s}$, unitary in the sense that $\boldsymbol{Q}^*\boldsymbol{G}\boldsymbol{Q} = \boldsymbol{I}_s$, and an upper triangular matrix $\boldsymbol{R} \in \mathbb{C}^{s\times s}$ with positive diagonal elements, such that

$$\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{R}.$$

Specifically,

$$\boldsymbol{Q} = [\,\boldsymbol{q}_1\,|\,\boldsymbol{q}_2\,|\,\cdots\,|\,\boldsymbol{q}_s\,], \quad \boldsymbol{R} = \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1s} \\ & r_{22} & \cdots & r_{2s} \\ & & \ddots & \vdots \\ & & & r_{ss} \end{bmatrix},$$

$$\langle \boldsymbol{q}_i, \boldsymbol{q}_j\rangle = \boldsymbol{q}_i^*\boldsymbol{G}\boldsymbol{q}_j = \delta_{ij} \quad \forall\, i, j,$$

$$r_{ij} = \langle \boldsymbol{q}_i, \boldsymbol{a}_j\rangle = \boldsymbol{q}_i^*\boldsymbol{G}\boldsymbol{a}_j \quad \forall\, i \leq j; \quad r_{ii} > 0 \quad \forall\, i.$$

In addition, the matrices $\boldsymbol{Q}$ and $\boldsymbol{R}$ are unique.

Concerning the computation of $\boldsymbol{Q}$ and $\boldsymbol{R}$ via the Gram–Schmidt and modified Gram–Schmidt orthogonalization, see the works mentioned above.

2 MPE and RRE redefined using a weighted inner product

2.1 General preliminaries

Let $\{\boldsymbol{x}_m\}$ be a vector sequence in $\mathbb{C}^N$. For the sake of argument, we may assume that this sequence results from the fixed-point iterative solution of the linear or nonlinear system of equations

$$\boldsymbol{x} = \boldsymbol{f}(\boldsymbol{x}), \quad \text{solution } \boldsymbol{s}; \quad \boldsymbol{x} \in \mathbb{C}^N \quad \text{and} \quad \boldsymbol{f} : \mathbb{C}^N \to \mathbb{C}^N, \tag{2.1}$$

that is, from

$$\boldsymbol{x}_{m+1} = \boldsymbol{f}(\boldsymbol{x}_m), \quad m = 0, 1, \ldots, \tag{2.2}$$

$\boldsymbol{x}_0$ being an initial vector chosen by the user. Normally, N is large and $\boldsymbol{f}(\boldsymbol{x})$ is a sparse vector-valued function. Now, when the sequence $\{\boldsymbol{x}_m\}$ converges, it does so to the solution $\boldsymbol{s}$, that is, $\lim_{m\to\infty} \boldsymbol{x}_m = \boldsymbol{s}$. In case $\{\boldsymbol{x}_m\}$ diverges, we call $\boldsymbol{s}$ the antilimit of $\{\boldsymbol{x}_m\}$; vector extrapolation methods in general, and MPE and RRE in particular, may produce sequences of approximations that converge to $\boldsymbol{s}$, the antilimit of $\{\boldsymbol{x}_m\}$, in such a case.

Let us define the vectors $\boldsymbol{u}_i$ via

$$\boldsymbol{u}_i = \boldsymbol{x}_{i+1} - \boldsymbol{x}_i, \quad i = 0, 1, \ldots, \tag{2.3}$$

and the $N \times (k+1)$ matrices $\boldsymbol{U}_k$ via

$$\boldsymbol{U}_k = [\,\boldsymbol{u}_0\,|\,\boldsymbol{u}_1\,|\,\cdots\,|\,\boldsymbol{u}_k\,], \quad k = 0, 1, \ldots. \tag{2.4}$$

Of course, there is an integer $k_0 \le N$, such that the matrices $\boldsymbol{U}_k$, $k = 0, 1, \ldots, k_0-1$, are of full rank, but $\boldsymbol{U}_{k_0}$ is not; that is,

$$\text{rank}\,(\boldsymbol{U}_k) = k+1, \quad k = 0, 1, \ldots, k_0-1; \quad \text{rank}\,(\boldsymbol{U}_{k_0}) = k_0. \tag{2.5}$$

(Of course, this is the same as saying that $\{\boldsymbol{u}_0, \boldsymbol{u}_1, \ldots, \boldsymbol{u}_{k_0-1}\}$ is a linearly independent set, but $\{\boldsymbol{u}_0, \boldsymbol{u}_1, \ldots, \boldsymbol{u}_{k_0}\}$ is not).

Then, both MPE and RRE produce approximations $\boldsymbol{s}_k$ (with $k \le k_0$) to the solution $\boldsymbol{s}$ of (2.1) that are of the form

$$\boldsymbol{s}_k = \sum_{i=0}^{k} \gamma_i \boldsymbol{x}_i; \quad \sum_{i=0}^{k} \gamma_i = 1, \tag{2.6}$$

for some scalars γ_i. On account of the condition $\sum_{i=0}^{k} \gamma_i = 1$, and because $\boldsymbol{x}_i = \boldsymbol{x}_0 + \sum_{j=0}^{i-1} \boldsymbol{u}_j$, we can rewrite (2.6) in the form

$$\boldsymbol{s}_k = \boldsymbol{x}_0 + \sum_{j=0}^{k-1} \xi_j \boldsymbol{u}_j; \quad \xi_j = \sum_{i=j+1}^{k} \gamma_i, \quad j = 0, 1, \ldots, k-1, \tag{2.7}$$

which can also be expressed in matrix terms as in

$$\boldsymbol{s}_k = \boldsymbol{x}_0 + \boldsymbol{U}_{k-1}\boldsymbol{\xi}, \quad \boldsymbol{\xi} = [\xi_0, \xi_1, \ldots, \xi_{k-1}]^T. \tag{2.8}$$

We will make use of both representations of $\boldsymbol{s}_k$, namely, (2.6) and (2.7)–(2.8), later. The γ_i and ξ_j for MPE are, of course, different from those for RRE, in general.

In the sequel, where confusion may arise, we will denote the vectors $\boldsymbol{s}_k$ resulting from MPE and RRE by $\boldsymbol{s}_k^{\text{MPE}}$ and $\boldsymbol{s}_k^{\text{RRE}}$, respectively. Similarly, to avoid confusion, we will denote the vectors $\boldsymbol{\gamma} = [\gamma_0, \gamma_1, \ldots, \gamma_k]^T$ and $\boldsymbol{\xi} = [\xi_0, \xi_1, \ldots, \xi_{k-1}]^T$ corresponding to $\boldsymbol{s}_k$ by $\boldsymbol{\gamma}_k$ (or $\boldsymbol{\gamma}_k^{\text{MPE}}$ or $\boldsymbol{\gamma}_k^{\text{RRE}}$) and $\boldsymbol{\xi}_k$ (or $\boldsymbol{\xi}_k^{\text{MPE}}$ or $\boldsymbol{\xi}_k^{\text{RRE}}$), respectively, depending on the context. When necessary, we will also denote (i) the γ_i associated with $\boldsymbol{\gamma}_k$ by γ_{ki} and (ii) the ξ_j associated with $\boldsymbol{\xi}_k$ by ξ_{kj} . That is,

$$\boldsymbol{\gamma}_k = [\gamma_{k0}, \ldots, \gamma_{kk}]^T \text{and } \boldsymbol{\xi}_k = [\xi_{k0}, \xi_{k1}, \ldots, \xi_{k,k-1}]^T.$$

We now describe how the γ_i for MPE and RRE are determined when these methods are defined within the context of $\mathbb{C}^N$ endowed with a weighted inner product and the norm induced by it.

2.2 Definition of the γ_i for MPE and RRE

2.2.1 The γ_i for MPE

Solve by least squares the linear overdetermined system of equations

$$\sum_{i=0}^{k-1} c_i \boldsymbol{u}_i = -\boldsymbol{u}_k \tag{2.9}$$

for $c_0, c_1, \ldots, c_{k-1}$. Clearly, this system can be expressed in matrix form as in

$$\boldsymbol{U}_{k-1}\boldsymbol{c}' = -\boldsymbol{u}_k; \quad \boldsymbol{c}' = [c_0, c_1, \ldots, c_{k-1}]^T, \tag{2.10}$$

and the least squares problem becomes

$$\min_{\boldsymbol{c}'} [\![\boldsymbol{U}_{k-1}\boldsymbol{c}' + \boldsymbol{u}_k]\!]. \tag{2.11}$$

Since $\boldsymbol{U}_{k-1}$ has full column rank, this problem has a unique solution for $\boldsymbol{c}'$. Next, set $c_k = 1$, and compute

$$\gamma_i = \frac{c_i}{\sum_{i=0}^{k} c_i}, \quad i = 0, 1, \ldots, k, \quad \text{provided} \quad \sum_{i=0}^{k} c_i \neq 0. \tag{2.12}$$

From this, we see that $\boldsymbol{s}_k$ for MPE exists and is unique if and only if $\sum_{i=0}^{k} c_i \neq 0$. (Of course, this means that $\boldsymbol{s}_k$ for MPE may fail to exist for some k in some cases).

2.2.2 *The γ_i for RRE*

Solve by least squares the linear overdetermined system of equations

$$\sum_{i=0}^{k} \gamma_i \boldsymbol{u}_i = \boldsymbol{0}, \tag{2.13}$$

subject to the constraint $\sum_{i=0}^{k} \gamma_i = 1$, for $\gamma_0, \gamma_1, \ldots, \gamma_k$. Clearly, this system too can be expressed in matrix form as in

$$\boldsymbol{U}_k \boldsymbol{\gamma} = \boldsymbol{0}, \quad \boldsymbol{\gamma} = [\gamma_0, \gamma_1, \ldots, \gamma_k]^T, \tag{2.14}$$

and the constrained least squares problem becomes

$$\min_{\boldsymbol{\gamma}} [\![\boldsymbol{U}_k \boldsymbol{\gamma}]\!], \quad \text{subject to} \quad \hat{\boldsymbol{e}}_k^T \boldsymbol{\gamma} = 1; \quad \hat{\boldsymbol{e}}_k = [1, 1, \ldots, 1]^T \in \mathbb{C}^{k+1}. \tag{2.15}$$

(Here $\hat{\boldsymbol{e}}_k$ should not be confused with the kth standard basis vector). Since $\boldsymbol{U}_k$ is of full column rank, this problem has a unique solution for $\boldsymbol{\gamma}$. From this, it is clear that $\boldsymbol{s}_k$ for RRE exists and is unique unconditionally.

2.3 The special case $k = k_0$

With $\boldsymbol{s}_k$ for MPE and RRE already defined, we start with a discussion of the case in which $k = k_0$.

Theorem 2.1 *Let $\{\boldsymbol{x}_m\}$ be an arbitrary sequence, and let MPE and RRE be as defined above.*

1. *Provided $\boldsymbol{s}_{k_0}^{\text{MPE}}$ exists, we have $\boldsymbol{s}_{k_0}^{\text{MPE}} = \boldsymbol{s}_{k_0}^{\text{RRE}}$.*
2. *Assume the sequence $\{\boldsymbol{x}_m\}$ is generated via (2.1) and (2.2) with a linear $\boldsymbol{f}(\boldsymbol{x})$, namely, with $\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{T}\boldsymbol{x} + \boldsymbol{d}$, where $\boldsymbol{T} \in \mathbb{C}^{N\times N}$ is some constant matrix and $\boldsymbol{d} \in \mathbb{C}^N$ is some constant vector, and $(\boldsymbol{I} - \boldsymbol{T})$ is nonsingular. Then $\boldsymbol{s}_{k_0}^{\text{MPE}}$ exists, and there holds $\boldsymbol{s}_{k_0}^{\text{MPE}} = \boldsymbol{s}_{k_0}^{\text{RRE}} = \boldsymbol{s}$, $\boldsymbol{s}$ being the (unique) solution to $\boldsymbol{x} = \boldsymbol{T}\boldsymbol{x} + \boldsymbol{d}$.*

In this case, k_0 is the degree of the minimal polynomial of $\boldsymbol{T}$ with respect to the vector $\boldsymbol{u}_0$.

Proof We start by observing that the matrix $\boldsymbol{U}_{k_0-1}$ has full rank and that the vector $\boldsymbol{u}_{k_0}$ is a linear combination of $\boldsymbol{u}_0, \boldsymbol{u}_1, \dots, \boldsymbol{u}_{k_0-1}$. As result, the linear system in (2.10) is consistent, hence has a unique solution for $\boldsymbol{c}'$ in the regular sense, this solution being also the solution to the minimization problem in (2.11). Letting $c_{k_0} = 1$ and proceeding as in (2.12), we obtain the $\boldsymbol{\gamma}^{\text{MPE}}_{k_0}$. A similar argument based on (2.14) and (2.15) shows that $\boldsymbol{\gamma}^{\text{RRE}}_{k_0} = \boldsymbol{\gamma}^{\text{MPE}}_{k_0}$. This proves part 1 of the theorem. Part 2 can be proved as in [32], for example. □

Since we already know the connection between $\boldsymbol{s}^{\text{MPE}}_{k_0}$ and $\boldsymbol{s}^{\text{RRE}}_{k_0}$, in the sequel, we will consider the cases in which $k < k_0$ strictly.

2.4 Determination of the γ_i via weighted QR factorization

A numerically stable and computationally economical algorithm for computing the γ_i for both MPE and RRE when $\boldsymbol{M} = \boldsymbol{I}$ has been given in Sidi [25]. A nice feature of this algorithm is that it proceeds via the QR factorization of the matrices $\boldsymbol{U}_k$ and unifies the treatments of MPE and RRE. Of course, in order to accommodate the weighted inner product $\langle\cdot,\cdot\rangle$ and the norm $[\![\cdot]\!]$ induced by it, we need a different algorithm. Interestingly, an algorithm that is very similar (in fact, identical in form) to the one developed in [25] can be formulated for this case. This can be accomplished by proceeding via the weighted QR factorization of $\boldsymbol{U}_k$. Even though this algorithm, just as that in [25], is designed for *computational* purposes, it turns out to be very useful for the *theoretical* study of this work concerning the relation between MPE and RRE. For some of the details concerning the developments that follow next, we refer the reader to [25].

We start with the weighted QR factorization of $\boldsymbol{U}_k$. Since $\boldsymbol{U}_k$ is of full column rank, by Theorem 1.1, it has a unique weighted QR factorization given as in

$$\boldsymbol{U}_k = \boldsymbol{Q}_k\boldsymbol{R}_k; \quad \boldsymbol{Q}_k \in \mathbb{C}^{N\times(k+1)}, \quad \boldsymbol{R}_k \in \mathbb{C}^{(k+1)\times(k+1)}, \tag{2.16}$$

where $\boldsymbol{Q}_k$ is unitary in the sense that $\boldsymbol{Q}_k^*\boldsymbol{M}\boldsymbol{Q}_k = \boldsymbol{I}_{k+1}$ since $k < N$, and $\boldsymbol{R}_k$ is upper triangular with positive diagonal elements; that is,

$$\boldsymbol{Q}_k = [\,\boldsymbol{q}_0\,|\,\boldsymbol{q}_1\,|\,\cdots\,|\,\boldsymbol{q}_k\,], \quad \boldsymbol{R}_k = \begin{bmatrix} r_{00} & r_{01} & \cdots & r_{0k} \\ & r_{11} & \cdots & r_{1k} \\ & & \ddots & \vdots \\ & & & r_{kk} \end{bmatrix}, \tag{2.17}$$

$$\boldsymbol{q}_i^*\boldsymbol{M}\boldsymbol{q}_j = \delta_{ij} \quad \forall\, i, j; \quad r_{ij} = \boldsymbol{q}_i^*\boldsymbol{M}\boldsymbol{u}_j \quad \forall\, i \le j; \quad r_{ii} > 0 \quad \forall\, i. \tag{2.18}$$

(Note that, having positive diagonal elements and being upper triangular, $\boldsymbol{R}_k$ is also nonsingular). Clearly, just as $\boldsymbol{U}_k$ has the partitioning $\boldsymbol{U}_k = [\boldsymbol{U}_{k-1}\,|\,\boldsymbol{u}_k\,]$, $\boldsymbol{Q}_k$ and $\boldsymbol{R}_k$

have the partitionings

$$\boldsymbol{Q}_k = [\boldsymbol{Q}_{k-1}\,|\,\boldsymbol{q}_k] \quad \text{and} \quad \boldsymbol{R}_k = \left[\begin{array}{c|c} \boldsymbol{R}_{k-1} & \boldsymbol{\rho}_k \\ \hline \boldsymbol{0}^T & r_{kk} \end{array}\right], \quad \boldsymbol{\rho}_k = [r_{0k}, r_{1k}, \ldots, r_{k-1,k}]^T. \tag{2.19}$$

We will make use of the following easily verifiable lemma in the sequel:

Lemma 2.2 *Let*

$$\boldsymbol{P} \in \mathbb{C}^{N\times j} \quad \textit{and} \quad \boldsymbol{P}^*\boldsymbol{M}\boldsymbol{P} = \boldsymbol{I}_j.$$

Then

$$\langle \boldsymbol{P}\boldsymbol{y}, \boldsymbol{P}\boldsymbol{z}\rangle = \boldsymbol{y}^*\boldsymbol{z} = (\boldsymbol{y}, \boldsymbol{z}) \quad \textit{and} \quad [\![\boldsymbol{P}\boldsymbol{z}]\!] = \sqrt{\boldsymbol{z}^*\boldsymbol{z}} = \|\boldsymbol{z}\|.$$

By this lemma, for arbitrary k, we have

$$\langle \boldsymbol{Q}_k\boldsymbol{y}, \boldsymbol{Q}_k\boldsymbol{z}\rangle = \boldsymbol{y}^*\boldsymbol{z} = (\boldsymbol{y}, \boldsymbol{z}) \quad \text{and} \quad [\![\boldsymbol{Q}_k\boldsymbol{z}]\!] = \sqrt{\boldsymbol{z}^*\boldsymbol{z}} = \|\boldsymbol{z}\| \tag{2.20}$$

and

$$[\![\boldsymbol{U}_k\boldsymbol{z}]\!] = \|\boldsymbol{R}_k\boldsymbol{z}\|. \tag{2.21}$$

Of these, (2.20) follows from $\boldsymbol{Q}_k^*\boldsymbol{M}\boldsymbol{Q}_k = \boldsymbol{I}_{k+1}$, while (2.21) follows from $\boldsymbol{U}_k = \boldsymbol{Q}_k\boldsymbol{R}_k$ and (2.20).

2.4.1 Determination of $\boldsymbol{\gamma}_k$ for MPE

Let us fix $c_k = 1$ and let $\boldsymbol{c} = [c_0, c_1, \ldots, c_k]^T = \left[\begin{array}{c} \boldsymbol{c}' \\ \hline 1 \end{array}\right]$. Then we have

$$\boldsymbol{U}_{k-1}\boldsymbol{c}' + \boldsymbol{u}_k = \boldsymbol{U}_k\boldsymbol{c} \quad \Rightarrow \quad [\![\boldsymbol{U}_{k-1}\boldsymbol{c}' + \boldsymbol{u}_k]\!] = [\![\boldsymbol{U}_k\boldsymbol{c}]\!] = \|\boldsymbol{R}_k\boldsymbol{c}\|,$$

and the minimization problem in (2.11) becomes,

$$\min_{\boldsymbol{c}'} \|\boldsymbol{R}_k\boldsymbol{c}\|.$$

By (2.19),

$$\boldsymbol{R}_k\boldsymbol{c} = \left[\begin{array}{c|c} \boldsymbol{R}_{k-1} & \boldsymbol{\rho}_k \\ \hline \boldsymbol{0}^T & r_{kk} \end{array}\right]\left[\begin{array}{c} \boldsymbol{c}' \\ \hline 1 \end{array}\right] = \left[\begin{array}{c} \boldsymbol{R}_{k-1}\boldsymbol{c}' + \boldsymbol{\rho}_k \\ \hline r_{kk} \end{array}\right], \tag{2.22}$$

which, upon taking norms, yields

$$\|\boldsymbol{R}_k\boldsymbol{c}\|^2 = \|\boldsymbol{R}_{k-1}\boldsymbol{c}' + \boldsymbol{\rho}_k\|^2 + r_{kk}^2.$$

Clearly, by the fact that $\boldsymbol{R}_{k-1}$ is a nonsingular $k \times k$ matrix, the minimum of $\|\boldsymbol{R}_k\boldsymbol{c}\|$ with respect to $\boldsymbol{c}'$ is achieved when $\boldsymbol{c}'$ satisfies

$$\boldsymbol{R}_{k-1}\boldsymbol{c}' + \boldsymbol{\rho}_k = \boldsymbol{0} \quad \Rightarrow \quad \boldsymbol{R}_{k-1}\boldsymbol{c}' = -\boldsymbol{\rho}_k \quad \Rightarrow \quad \boldsymbol{c}' = -\boldsymbol{R}_{k-1}^{-1}\boldsymbol{\rho}_k. \tag{2.23}$$

Of course, $\boldsymbol{c}'$ is unique, and so is $\boldsymbol{c}$.

With $\boldsymbol{c}' = -\boldsymbol{R}_{k-1}^{-1}\boldsymbol{\rho}_k$, the vector $\boldsymbol{\gamma}_k$ in MPE is obtained as in

$$\boldsymbol{\gamma}_k^{\text{MPE}} = \frac{\boldsymbol{c}}{\hat{\boldsymbol{e}}_k^T\boldsymbol{c}}, \quad \boldsymbol{c} = \left[\begin{array}{c} \boldsymbol{c}' \\ \hline 1 \end{array}\right]. \tag{2.24}$$

Of course, this is valid only when $\hat{\boldsymbol{e}}_k^T\boldsymbol{c} = \sum_{i=0}^k c_i \neq 0$, hence only when $\boldsymbol{s}_k^{\text{MPE}}$ exists. The vector $\boldsymbol{c}$ exists uniquely whether $\boldsymbol{s}_k^{\text{MPE}}$ exists or not, however.

2.4.2 Determination of $\boldsymbol{\gamma}_k$ for RRE

By the fact that $[\![\boldsymbol{U}_k\boldsymbol{y}]\!] = \|\boldsymbol{R}_k\boldsymbol{y}\|$, the minimization problem in (2.15) becomes

$$\min_{\boldsymbol{\gamma}} \|\boldsymbol{R}_k\boldsymbol{\gamma}\|, \quad \text{subject to} \quad \hat{\boldsymbol{e}}_k^T\boldsymbol{\gamma} = 1,$$

and equivalently,

$$\min_{\boldsymbol{\gamma}} \boldsymbol{\gamma}^*(\boldsymbol{R}_k^*\boldsymbol{R}_k)\boldsymbol{\gamma}, \quad \text{subject to} \quad \hat{\boldsymbol{e}}_k^T\boldsymbol{\gamma} = 1.$$

By the lemma in [25, Appendix A], the solution for the vector $\boldsymbol{\gamma}_k$ in RRE proceeds through the following steps:

$$\boldsymbol{R}_k^*\boldsymbol{R}_k\boldsymbol{h} = \hat{\boldsymbol{e}}_k, \quad \boldsymbol{h} = [h_0, h_1, \dots, h_k]^T \quad (\text{solve for } \boldsymbol{h}). \tag{2.25}$$

$$\lambda = \frac{1}{\sum_{i=0}^k h_i} = \frac{1}{\hat{\boldsymbol{e}}_k^T\boldsymbol{h}} \quad (\lambda > 0 \text{ always}). \tag{2.26}$$

$$\boldsymbol{\gamma}_k^{\text{RRE}} = \lambda\boldsymbol{h}. \tag{2.27}$$

Note that $\boldsymbol{h}$ can be determined by solving two $(k+1)$-dimensional triangular linear systems, namely, (i) $\boldsymbol{R}_k^*\boldsymbol{y} = \hat{\boldsymbol{e}}_k$ for $\boldsymbol{y}$ and (ii) $\boldsymbol{R}_k\boldsymbol{h} = \boldsymbol{y}$ for $\boldsymbol{h}$.

For our theoretical study, we need to have $\boldsymbol{\gamma}_k$ in analytical form. This is achieved as follows: Substituting $\boldsymbol{h} = (\boldsymbol{R}_k^*\boldsymbol{R}_k)^{-1}\hat{\boldsymbol{e}}_k$ from (2.25) in (2.26) and (2.27), we have

$$\lambda = \frac{1}{\hat{\boldsymbol{e}}_k^T(\boldsymbol{R}_k^*\boldsymbol{R}_k)^{-1}\hat{\boldsymbol{e}}_k} = \frac{1}{\|\boldsymbol{R}_k^{-*}\hat{\boldsymbol{e}}_k\|^2} \tag{2.28}$$

and

$$\boldsymbol{\gamma}_k^{\text{RRE}} = \frac{(\boldsymbol{R}_k^*\boldsymbol{R}_k)^{-1}\hat{\boldsymbol{e}}_k}{\hat{\boldsymbol{e}}_k^T(\boldsymbol{R}_k^*\boldsymbol{R}_k)^{-1}\hat{\boldsymbol{e}}_k} = \frac{\boldsymbol{R}_k^{-1}(\boldsymbol{R}_k^{-*}\hat{\boldsymbol{e}}_k)}{\|\boldsymbol{R}_k^{-*}\hat{\boldsymbol{e}}_k\|^2}. \tag{2.29}$$

[Here and in the sequel, $\boldsymbol{B}^{-*}$ stands for $(\boldsymbol{B}^*)^{-1} = (\boldsymbol{B}^{-1})^*$].

2.5 Unified algorithm for MPE and RRE

Once the $\boldsymbol{\gamma}_k$ have been computed as described above, the computation of $\boldsymbol{s}_k$ can be achieved via (2.7)–(2.8) as follows: First, we compute the vector $\boldsymbol{\xi}_k = [\xi_0, \xi_1, \dots, \xi_k]^T$ via (2.7), and then, by invoking $\boldsymbol{U}_{k-1} = \boldsymbol{Q}_{k-1}\boldsymbol{R}_{k-1}$, we compute $\boldsymbol{s}_k$ via (2.8), as in

$$\boldsymbol{s}_k = \boldsymbol{x}_0 + \boldsymbol{Q}_{k-1}(\boldsymbol{R}_{k-1}\boldsymbol{\xi}_k) = \boldsymbol{x}_0 + \sum_{i=0}^{k-1}\eta_i\boldsymbol{q}_i;$$

$$\boldsymbol{\eta} = \boldsymbol{R}_{k-1}\boldsymbol{\xi}_k, \quad \boldsymbol{\eta} = [\eta_0, \eta_1, \dots, \eta_{k-1}]^T. \tag{2.30}$$

For convenience, we give a complete description of the unified algorithm in Table 1.

2.6 Error assessment

Let us now return to the system of equations in (2.1). If $\boldsymbol{x}$ is an approximation to the solution $\boldsymbol{s}$ of this system, then one good measure of the accuracy of

Table 1 Unified algorithm for implementing MPE and RRE

Step 0. Input: The hermitian positive definite matrix $\boldsymbol{M} \in \mathbb{C}^{N\times N}$, the integer k, and the vectors $\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_{k+1}$.

Step 1. Compute $\boldsymbol{u}_i = \Delta\boldsymbol{x}_i = \boldsymbol{x}_{i+1} - \boldsymbol{x}_i,\ \ i = 0, 1, \ldots, k$.
Set $\boldsymbol{U}_j = [\boldsymbol{u}_0\,|\,\boldsymbol{u}_1\,|\,\cdots\,|\,\boldsymbol{u}_j] \in \mathbb{C}^{N\times(j+1)},\ \ j = 0, 1, \ldots$.
Compute the weighted QR factorization of $\boldsymbol{U}_k$, namely, $\boldsymbol{U}_k = \boldsymbol{Q}_k\boldsymbol{R}_k$;
$\boldsymbol{Q}_k = [\boldsymbol{q}_0\,|\,\boldsymbol{q}_1\,|\,\cdots\,|\,\boldsymbol{q}_k]$ unitary in the sense $\boldsymbol{Q}_k^*\boldsymbol{M}\boldsymbol{Q}_k = \boldsymbol{I}_{k+1}$, and
$\boldsymbol{R}_k = [r_{ij}]_{0\le i,j\le k}$ upper triangular, $r_{ij} = \boldsymbol{q}_i^*\boldsymbol{M}\boldsymbol{u}_j$.
($\boldsymbol{U}_{k-1} = \boldsymbol{Q}_{k-1}\boldsymbol{R}_{k-1}$ is contained in $\boldsymbol{U}_k = \boldsymbol{Q}_k\boldsymbol{R}_k$).

Step 2. Computation of $\boldsymbol{\gamma}_k = [\gamma_0, \gamma_1, \ldots, \gamma_k]^T$:

For MPE:
Solve the (upper triangular) linear system

$$\boldsymbol{R}_{k-1}\boldsymbol{c}' = -\boldsymbol{\rho}_k; \quad \boldsymbol{\rho}_k = [r_{0k}, r_{1k}, \ldots, r_{k-1,k}]^T, \quad \boldsymbol{c}' = [c_0, c_1, \ldots, c_{k-1}]^T.$$

(Note that $\boldsymbol{\rho}_k = \boldsymbol{Q}_{k-1}^*\boldsymbol{M}\boldsymbol{u}_k$).
Set $c_k = 1$ and compute $\alpha = \sum_{i=0}^{k} c_i$.
Set $\boldsymbol{\gamma}_k = \boldsymbol{c}/\alpha$; that is, $\gamma_i = c_i/\alpha,\ \ i = 0, 1, \ldots, k$, provided $\alpha \neq 0$.

For RRE:
Solve the linear system

$$\boldsymbol{R}_k^*\boldsymbol{R}_k\boldsymbol{h} = \hat{\boldsymbol{e}}_k; \quad \boldsymbol{h} = [h_0, h_1, \ldots, h_k]^T, \quad \hat{\boldsymbol{e}}_k = [1, 1, \ldots, 1]^T \in \mathbb{C}^{k+1}.$$

[This amounts to solving two triangular (lower and upper) systems].
Set $\lambda = \left(\sum_{i=0}^{k} h_i\right)^{-1}$. (Note that λ is real and positive).
Set $\boldsymbol{\gamma}_k = \lambda\boldsymbol{h}$; that is, $\gamma_i = \lambda h_i,\ \ i = 0, 1, \ldots, k$.

Step 3. Compute $\boldsymbol{\xi}_k = [\xi_0, \xi_1, \ldots, \xi_{k-1}]^T$ by

$$\xi_0 = 1 - \gamma_0; \quad \xi_j = \xi_{j-1} - \gamma_j, \quad j = 1, \ldots, k-1.$$

Compute $\boldsymbol{s}_k^{MPE}$ and $\boldsymbol{s}_k^{RRE}$ via

$$\boldsymbol{s}_k = \boldsymbol{x}_0 + \boldsymbol{Q}_{k-1}\big(\boldsymbol{R}_{k-1}\boldsymbol{\xi}_k\big) = \boldsymbol{x}_0 + \boldsymbol{Q}_{k-1}\boldsymbol{\eta}.$$

[For this, first compute $\boldsymbol{\eta} = \boldsymbol{R}_{k-1}\boldsymbol{\xi}_k,\ \ \boldsymbol{\eta} = [\eta_0, \eta_1, \ldots, \eta_{k-1}]^T$.
Next, set $\boldsymbol{s}_k = \boldsymbol{x}_0 + \sum_{i=0}^{k-1}\eta_i\boldsymbol{q}_i$].

$\boldsymbol{x}$ is (some norm of) the residual vector $\boldsymbol{r}(\boldsymbol{x})$ corresponding to $\boldsymbol{x}$ that is given by

$$\boldsymbol{r}(\boldsymbol{x}) = \boldsymbol{f}(\boldsymbol{x}) - \boldsymbol{x}. \tag{2.31}$$

This is natural because $\lim_{\boldsymbol{x}\to\boldsymbol{s}}\boldsymbol{r}(\boldsymbol{x}) = \boldsymbol{r}(\boldsymbol{s}) = \boldsymbol{0}$. In case the sequence $\{\boldsymbol{x}_m\}$ is being generated as in (2.2) for solving (2.1), our measure for the quality of $\boldsymbol{s}_k$ will then be $\boldsymbol{r}(\boldsymbol{s}_k)$. The following have been shown in [25]:

- When $\boldsymbol{f}(\boldsymbol{x})$ is linear [that is, $\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{T}\boldsymbol{x} + \boldsymbol{d}$ for some constant matrix $\boldsymbol{T} \in \mathbb{C}^{N\times N}$ and constant vector $\boldsymbol{d} \in \mathbb{C}^{N}$], $\boldsymbol{r}(\boldsymbol{s}_k) = \boldsymbol{U}_k\boldsymbol{\gamma}_k$ *exactly*.
- When $\boldsymbol{f}(\boldsymbol{x})$ is nonlinear, $\boldsymbol{U}_k\boldsymbol{\gamma}_k$ serves as an *approximation* to $\boldsymbol{r}(\boldsymbol{s}_k)$, that is, $\boldsymbol{r}(\boldsymbol{s}_k) \approx \boldsymbol{U}_k\boldsymbol{\gamma}_k$,and $\boldsymbol{U}_k\boldsymbol{\gamma}_k$ gets closer and closer to $\boldsymbol{r}(\boldsymbol{s}_k)$ as convergence is approached.

In addition, $[\![\boldsymbol{U}_k\boldsymbol{\gamma}_k]\!]$, the weighted norm of $\boldsymbol{U}_k\boldsymbol{\gamma}_k$, can be obtained, without actually computing $\boldsymbol{U}_k\boldsymbol{\gamma}_k$ and taking its norm, in terms of the quantities provided by the algorithm we have just described. This is the subject of the next theorem.

Theorem 2.3 *The vectors $\boldsymbol{U}_k\boldsymbol{\gamma}_k^{\text{MPE}}$ and $\boldsymbol{U}_k\boldsymbol{\gamma}_k^{\text{RRE}}$ satisfy*

$$[\![\boldsymbol{U}_k\boldsymbol{\gamma}_k^{\text{MPE}}]\!] = r_{kk}|\gamma_k| \quad \textit{and} \quad [\![\boldsymbol{U}_k\boldsymbol{\gamma}_k^{\text{RRE}}]\!] = \sqrt{\lambda}. \tag{2.32}$$

Remarks.

1. Of course, γ_k in (2.32) is γ_{kk}^{MPE}, namely, the last component of the vector $\boldsymbol{\gamma}_k^{\text{MPE}}$ corresponding to $\boldsymbol{s}_k^{\text{MPE}}$. Similarly, λ in (2.32) is as defined in (2.26) for $\boldsymbol{s}_k^{\text{RRE}}$.
2. Clearly, (2.32) is valid for *all* sequences $\{\boldsymbol{x}_m\}$, whether these are generated by a (linear or nonlinear) fixed-point iterative scheme or otherwise.

Proof By (2.21), we have that $[\![\boldsymbol{U}_k\boldsymbol{\gamma}_k]\!] = \|\boldsymbol{R}_k\boldsymbol{\gamma}_k\|$. Therefore, it is enough to look at $\|\boldsymbol{R}_k\boldsymbol{\gamma}_k^{\text{MPE}}\|$ and $\|\boldsymbol{R}_k\boldsymbol{\gamma}_k^{\text{RRE}}\|$.

For MPE, by (2.22), (2.23), and (2.24), with $\gamma_k = 1/\hat{\boldsymbol{e}}_k^T\boldsymbol{c}$, we have

$$\boldsymbol{R}_k\boldsymbol{\gamma}_k^{\text{MPE}} = \frac{1}{\hat{\boldsymbol{e}}_k^T\boldsymbol{c}}(\boldsymbol{R}_k\boldsymbol{c}) = \gamma_k\begin{bmatrix}\boldsymbol{0}\\ \hline r_{kk}\end{bmatrix} = r_{kk}\gamma_k\begin{bmatrix}\boldsymbol{0}\\ \hline 1\end{bmatrix}.$$

Taking norms on both sides, we obtain the result for MPE.

As for RRE, by (2.29), we have

$$\boldsymbol{R}_k\boldsymbol{\gamma}_k^{\text{RRE}} = \frac{\boldsymbol{R}_k^{-*}\hat{\boldsymbol{e}}_k}{\|\boldsymbol{R}_k^{-*}\hat{\boldsymbol{e}}_k\|^2}.$$

Taking norms on both sides, and invoking (2.28), we obtain the result for RRE. □

3 MPE and RRE are related

We begin by restating that since

$$\boldsymbol{U}_k\boldsymbol{\gamma}_k = \boldsymbol{Q}_k(\boldsymbol{R}_k\boldsymbol{\gamma}_k) \quad \text{and} \quad [\![\boldsymbol{U}_k\boldsymbol{\gamma}_k]\!] = \|\boldsymbol{R}_k\boldsymbol{\gamma}_k\|, \tag{3.1}$$

and since $\boldsymbol{Q}_k$ and $\boldsymbol{R}_k$ are the same for both MPE and RRE, the vector that is of relevance for both methods is $\boldsymbol{R}_k\boldsymbol{\gamma}_k$, and we turn to the study of this vector. In addition, we express everything in terms of the vectors $\boldsymbol{c}'$ and $\boldsymbol{c}$ and the matrices $\boldsymbol{Q}_k$ and $\boldsymbol{R}_k$, which do not depend either on $\boldsymbol{s}_k^{\text{MPE}}$ or $\boldsymbol{s}_k^{\text{RRE}}$. In the developments that follow, we will also recall that $\|\boldsymbol{y}\| = \sqrt{\boldsymbol{y}^*\boldsymbol{y}}$ always.

3.1 $\boldsymbol{R}_k\boldsymbol{\gamma}_k$ for MPE and RRE and an identity

Assuming that $\boldsymbol{s}_k^{\text{MPE}}$ exists, hence $\hat{\boldsymbol{e}}_k^T\boldsymbol{c} \neq 0$, by (2.24), we first have

$$\boldsymbol{R}_k\boldsymbol{\gamma}_k^{\text{MPE}} = \frac{1}{\hat{\boldsymbol{e}}_k^T\boldsymbol{c}}\boldsymbol{R}_k\boldsymbol{c},$$

which, upon invoking (2.22) and (2.23), becomes

$$\boldsymbol{R}_k\boldsymbol{\gamma}_k^{\text{MPE}} = \frac{r_{kk}}{\hat{\boldsymbol{e}}_k^T\boldsymbol{c}}\left[\frac{\boldsymbol{0}}{1}\right]. \tag{3.2}$$

Of course, this immediately implies that

$$\|\boldsymbol{R}_k\boldsymbol{\gamma}_k^{\text{MPE}}\| = \frac{r_{kk}}{|\hat{\boldsymbol{e}}_k^T\boldsymbol{c}|}. \tag{3.3}$$

As for RRE, by (2.29), we have

$$\boldsymbol{R}_k\boldsymbol{\gamma}_k^{\text{RRE}} = \frac{\boldsymbol{R}_k^{-*}\hat{\boldsymbol{e}}_k}{\|\boldsymbol{R}_k^{-*}\hat{\boldsymbol{e}}_k\|^2}. \tag{3.4}$$

Of course, this immediately implies that

$$\|\boldsymbol{R}_k\boldsymbol{\gamma}_k^{\text{RRE}}\| = \frac{1}{\|\boldsymbol{R}_k^{-*}\hat{\boldsymbol{e}}_k\|} \quad \Rightarrow \quad \boldsymbol{R}_k^{-*}\hat{\boldsymbol{e}}_k = \frac{\boldsymbol{R}_k\boldsymbol{\gamma}_k^{\text{RRE}}}{\|\boldsymbol{R}_k\boldsymbol{\gamma}_k^{\text{RRE}}\|^2}. \tag{3.5}$$

We now go on to study $\boldsymbol{R}_k^{-*}\hat{\boldsymbol{e}}_k$ in more detail. First, by (2.19) and (2.23),

$$\boldsymbol{R}_k^{-1} = \left[\begin{array}{c|c} \boldsymbol{R}_{k-1}^{-1} & \boldsymbol{c}'/r_{kk} \\ \hline \boldsymbol{0}^T & 1/r_{kk} \end{array}\right] \quad \Rightarrow \quad \boldsymbol{R}_k^{-*} = \left[\begin{array}{c|c} \boldsymbol{R}_{k-1}^{-*} & \boldsymbol{0} \\ \hline \boldsymbol{c}'^*/r_{kk} & 1/r_{kk} \end{array}\right]. \tag{3.6}$$

Consequently, invoking also $\hat{\boldsymbol{e}}_k = \left[\frac{\hat{\boldsymbol{e}}_{k-1}}{1}\right]$, we have

$$\begin{aligned} \boldsymbol{R}_k^{-*}\hat{\boldsymbol{e}}_k &= \left[\begin{array}{c|c} \boldsymbol{R}_{k-1}^{-*} & \boldsymbol{0} \\ \hline \boldsymbol{c}'^*/r_{kk} & 1/r_{kk} \end{array}\right]\left[\frac{\hat{\boldsymbol{e}}_{k-1}}{1}\right] \\ &= \left[\frac{\boldsymbol{R}_{k-1}^{-*}\hat{\boldsymbol{e}}_{k-1}}{\boldsymbol{c}'^*\hat{\boldsymbol{e}}_{k-1}/r_{kk} + 1/r_{kk}}\right] \\ &= \left[\frac{\boldsymbol{R}_{k-1}^{-*}\hat{\boldsymbol{e}}_{k-1}}{\overline{\hat{\boldsymbol{e}}_k^T\boldsymbol{c}}/r_{kk}}\right], \end{aligned} \tag{3.7}$$

which, by (3.5), can also be expressed as in

$$\frac{1}{\|\boldsymbol{R}_k\boldsymbol{\gamma}_k^{\text{RRE}}\|^2}\boldsymbol{R}_k\boldsymbol{\gamma}_k^{\text{RRE}} = \frac{1}{\|\boldsymbol{R}_{k-1}\boldsymbol{\gamma}_{k-1}^{\text{RRE}}\|^2}\left[\frac{\boldsymbol{R}_{k-1}\boldsymbol{\gamma}_{k-1}^{\text{RRE}}}{0}\right] + \frac{\overline{\hat{\boldsymbol{e}}_k^T\boldsymbol{c}}}{r_{kk}}\left[\frac{\boldsymbol{0}}{1}\right]. \tag{3.8}$$

Clearly, (3.8) is an *identity* for RRE relating $\boldsymbol{s}_{k-1}^{\text{RRE}}$ and $\boldsymbol{s}_k^{\text{RRE}}$; we will make use of it in the developments of the next subsection. (Here $\bar{t}$ stands for the complex conjugate of t).

Remark. Recall that the vector $\boldsymbol{c}$ exists uniquely for all $k < k_0$. Thus, (3.8) is valid whether $\boldsymbol{s}_k^{\text{MPE}}$ exists or not.

3.2 Main results

The following theorem is our first main result, and concerns the case in which $\boldsymbol{s}_k^{\text{MPE}}$ does not exist and RRE stagnates.

Theorem 3.1 1. *In case $\boldsymbol{s}_k^{\text{MPE}}$ does not exist, there holds*

$$\boldsymbol{s}_k^{\text{RRE}} = \boldsymbol{s}_{k-1}^{\text{RRE}}, \tag{3.9}$$

which also implies

$$\boldsymbol{U}_k \boldsymbol{\gamma}_k^{\text{RRE}} = \boldsymbol{U}_{k-1} \boldsymbol{\gamma}_{k-1}^{\text{RRE}}. \tag{3.10}$$

2. *Conversely, if (3.9) holds, then $\boldsymbol{s}_k^{\text{MPE}}$ does not exist.*

Proof The proof is based on the fact that $\boldsymbol{s}_k^{\text{MPE}}$ exists if and only if $\hat{\boldsymbol{e}}_k^T \boldsymbol{c} \neq 0$.
Proof of part 1: Since $\hat{\boldsymbol{e}}_k^T \boldsymbol{c} = 0$ when $\boldsymbol{s}_k^{\text{MPE}}$ does not exist, by (3.8),

$$\frac{1}{\|\boldsymbol{R}_k \boldsymbol{\gamma}_k^{\text{RRE}}\|^2} \boldsymbol{R}_k \boldsymbol{\gamma}_k^{\text{RRE}} = \frac{1}{\|\boldsymbol{R}_{k-1} \boldsymbol{\gamma}_{k-1}^{\text{RRE}}\|^2} \left[\frac{\boldsymbol{R}_{k-1} \boldsymbol{\gamma}_{k-1}^{\text{RRE}}}{0} \right]. \tag{3.11}$$

Taking Euclidean norms in (3.11), we obtain

$$\|\boldsymbol{R}_k \boldsymbol{\gamma}_k^{\text{RRE}}\| = \|\boldsymbol{R}_{k-1} \boldsymbol{\gamma}_{k-1}^{\text{RRE}}\|, \tag{3.12}$$

which, upon substituting back in (3.11), gives

$$\boldsymbol{R}_k \boldsymbol{\gamma}_k^{\text{RRE}} = \left[\frac{\boldsymbol{R}_{k-1} \boldsymbol{\gamma}_{k-1}^{\text{RRE}}}{0} \right] = \boldsymbol{R}_k \left[\frac{\boldsymbol{\gamma}_{k-1}^{\text{RRE}}}{0} \right]. \tag{3.13}$$

By the fact that $\boldsymbol{R}_k$ is nonsingular, it follows that

$$\boldsymbol{\gamma}_k^{\text{RRE}} = \left[\frac{\boldsymbol{\gamma}_{k-1}^{\text{RRE}}}{0} \right], \tag{3.14}$$

which, together with (2.6), gives (3.9).

Proof of part 2: By (3.9) and (2.8), we have

$$\boldsymbol{s}_k^{\text{RRE}} = \boldsymbol{x}_0 + \boldsymbol{U}_{k-1} \boldsymbol{\xi}_k^{\text{RRE}} = \boldsymbol{x}_0 + \boldsymbol{U}_{k-2} \boldsymbol{\xi}_{k-1}^{\text{RRE}} = \boldsymbol{s}_{k-1}^{\text{RRE}}, \tag{3.15}$$

from which

$$\boldsymbol{U}_{k-1} \boldsymbol{\xi}_k^{\text{RRE}} = \boldsymbol{U}_{k-2} \boldsymbol{\xi}_{k-1}^{\text{RRE}} \quad \Rightarrow \quad \boldsymbol{U}_{k-1} \boldsymbol{\xi}_k^{\text{RRE}} = \boldsymbol{U}_{k-1} \left[\frac{\boldsymbol{\xi}_{k-1}^{\text{RRE}}}{0} \right]. \tag{3.16}$$

By the fact that $\boldsymbol{U}_{k-1}$ is of full column rank, (3.16) implies that

$$\boldsymbol{\xi}_k^{\text{RRE}} = \left[\frac{\boldsymbol{\xi}_{k-1}^{\text{RRE}}}{0} \right], \tag{3.17}$$

which, when combined with the relation [$\xi_{kj} = \sum_{i=j+1}^{k} \gamma_{ki}$, by which, $\xi_{k,k-1} = \gamma_{kk}$] in (2.7), gives (3.14). Multiplying both sides of (3.14) on the left by $\boldsymbol{R}_k$, we obtain

$$\boldsymbol{R}_k \boldsymbol{\gamma}_k^{\text{RRE}} = \left[\frac{\boldsymbol{R}_{k-1} \boldsymbol{\gamma}_{k-1}^{\text{RRE}}}{0} \right] \quad \Rightarrow \quad \|\boldsymbol{R}_k \boldsymbol{\gamma}_k^{\text{RRE}}\| = \|\boldsymbol{R}_{k-1} \boldsymbol{\gamma}_{k-1}^{\text{RRE}}\|. \tag{3.18}$$

Substituting (3.18) in (3.8), we obtain $\hat{\boldsymbol{e}}_k^T \boldsymbol{c} = 0$, and this completes the proof. □

Remark. What Theorem 3.1 is saying is that the stagnation of RRE (in the sense that $\boldsymbol{s}_k^{\text{RRE}} = \boldsymbol{s}_{k-1}^{\text{RRE}}$) and the failure of $\boldsymbol{s}_k^{\text{MPE}}$ to exist take place simultaneously. In addition, this phenomenon is of a universal nature because it is independent of how the sequence $\{\boldsymbol{x}_m\}$ is generated.

The next theorem is our second main result, and concerns the general case in which $\boldsymbol{s}_k^{\text{MPE}}$ exists.

Theorem 3.2 *In case $\boldsymbol{s}_k^{\text{MPE}}$ exists, there hold*

$$\frac{1}{[\![\boldsymbol{U}_k\boldsymbol{\gamma}_k^{\text{RRE}}]\!]^2} = \frac{1}{[\![\boldsymbol{U}_{k-1}\boldsymbol{\gamma}_{k-1}^{\text{RRE}}]\!]^2} + \frac{1}{[\![\boldsymbol{U}_k\boldsymbol{\gamma}_k^{\text{MPE}}]\!]^2} \tag{3.19}$$

and

$$\frac{\boldsymbol{U}_k\boldsymbol{\gamma}_k^{\text{RRE}}}{[\![\boldsymbol{U}_k\boldsymbol{\gamma}_k^{\text{RRE}}]\!]^2} = \frac{\boldsymbol{U}_{k-1}\boldsymbol{\gamma}_{k-1}^{\text{RRE}}}{[\![\boldsymbol{U}_{k-1}\boldsymbol{\gamma}_{k-1}^{\text{RRE}}]\!]^2} + \frac{\boldsymbol{U}_k\boldsymbol{\gamma}_k^{\text{MPE}}}{[\![\boldsymbol{U}_k\boldsymbol{\gamma}_k^{\text{MPE}}]\!]^2}. \tag{3.20}$$

Consequently, we also have

$$\frac{\boldsymbol{s}_k^{\text{RRE}}}{[\![\boldsymbol{U}_k\boldsymbol{\gamma}_k^{\text{RRE}}]\!]^2} = \frac{\boldsymbol{s}_{k-1}^{\text{RRE}}}{[\![\boldsymbol{U}_{k-1}\boldsymbol{\gamma}_{k-1}^{\text{RRE}}]\!]^2} + \frac{\boldsymbol{s}_k^{\text{MPE}}}{[\![\boldsymbol{U}_k\boldsymbol{\gamma}_k^{\text{MPE}}]\!]^2}. \tag{3.21}$$

In addition,

$$[\![\boldsymbol{U}_k\boldsymbol{\gamma}_k^{\text{RRE}}]\!] < [\![\boldsymbol{U}_{k-1}\boldsymbol{\gamma}_{k-1}^{\text{RRE}}]\!]. \tag{3.22}$$

Proof Since $\boldsymbol{s}_k^{\text{MPE}}$ exists, we have $\hat{\boldsymbol{e}}_k^T \boldsymbol{c} \neq 0$. Taking the Euclidean norm of both sides in (3.8), and observing that the two terms on the right-hand side are orthogonal to each other in the Euclidean inner product, we first obtain

$$\frac{1}{\|\boldsymbol{R}_k\boldsymbol{\gamma}_k^{\text{RRE}}\|^2} = \frac{1}{\|\boldsymbol{R}_{k-1}\boldsymbol{\gamma}_{k-1}^{\text{RRE}}\|^2} + \left(\frac{|\hat{\boldsymbol{e}}_k^T \boldsymbol{c}|}{r_{kk}}\right)^2, \tag{3.23}$$

which, upon invoking (3.3), gives

$$\frac{1}{\|\boldsymbol{R}_k\boldsymbol{\gamma}_k^{\text{RRE}}\|^2} = \frac{1}{\|\boldsymbol{R}_{k-1}\boldsymbol{\gamma}_{k-1}^{\text{RRE}}\|^2} + \frac{1}{\|\boldsymbol{R}_k\boldsymbol{\gamma}_k^{\text{MPE}}\|^2}. \tag{3.24}$$

The result in (3.19) follows from (3.24) and (3.1).

Next, invoking (3.2) and (3.3) in (3.8), we obtain

$$\frac{1}{\|\boldsymbol{R}_k\boldsymbol{\gamma}_k^{\text{RRE}}\|^2}\boldsymbol{R}_k\boldsymbol{\gamma}_k^{\text{RRE}} = \frac{1}{\|\boldsymbol{R}_{k-1}\boldsymbol{\gamma}_{k-1}^{\text{RRE}}\|^2}\left[\frac{\boldsymbol{R}_{k-1}\boldsymbol{\gamma}_{k-1}^{\text{RRE}}}{0}\right] + \frac{1}{\|\boldsymbol{R}_k\boldsymbol{\gamma}_k^{\text{MPE}}\|^2}\boldsymbol{R}_k\boldsymbol{\gamma}_k^{\text{MPE}}. \tag{3.25}$$

Multiplying both sides of (3.25) on the left by $\boldsymbol{Q}_k$, and invoking (3.1) and

$$\boldsymbol{Q}_k\left[\frac{\boldsymbol{R}_{k-1}\boldsymbol{\gamma}_{k-1}^{\text{RRE}}}{0}\right] = [\,\boldsymbol{Q}_{k-1}\,|\,\boldsymbol{q}_k\,]\left[\frac{\boldsymbol{R}_{k-1}\boldsymbol{\gamma}_{k-1}^{\text{RRE}}}{0}\right] = \boldsymbol{Q}_{k-1}(\boldsymbol{R}_{k-1}\boldsymbol{\gamma}_{k-1}^{\text{RRE}}) = \boldsymbol{U}_{k-1}\boldsymbol{\gamma}_{k-1}^{\text{RRE}}, \tag{3.26}$$

we obtain (3.20).

Let us rewrite (3.20) in the form

$$\frac{1}{[\![\boldsymbol{U}_k\boldsymbol{\gamma}_k^{RRE}]\!]^2}\boldsymbol{U}_k\boldsymbol{\gamma}_k^{RRE}=\frac{1}{[\![\boldsymbol{U}_{k-1}\boldsymbol{\gamma}_{k-1}^{RRE}]\!]^2}\boldsymbol{U}_k\begin{bmatrix}\boldsymbol{\gamma}_{k-1}^{RRE}\\0\end{bmatrix}+\frac{1}{[\![\boldsymbol{U}_k\boldsymbol{\gamma}_k^{MPE}]\!]^2}\boldsymbol{U}_k\boldsymbol{\gamma}_k^{MPE}. \tag{3.27}$$

From (3.27) and by the fact that $\boldsymbol{U}_k$ is of full column rank, it follows that

$$\frac{1}{[\![\boldsymbol{U}_k\boldsymbol{\gamma}_k^{RRE}]\!]^2}\boldsymbol{\gamma}_k^{RRE}=\frac{1}{[\![\boldsymbol{U}_{k-1}\boldsymbol{\gamma}_{k-1}^{RRE}]\!]^2}\begin{bmatrix}\boldsymbol{\gamma}_{k-1}^{RRE}\\0\end{bmatrix}+\frac{1}{[\![\boldsymbol{U}_k\boldsymbol{\gamma}_k^{MPE}]\!]^2}\boldsymbol{\gamma}_k^{MPE}, \tag{3.28}$$

and this, together with (2.6), gives (3.21).

Finally, (3.22) follows directly from (3.19). □

The following facts can be deduced directly from (3.19):

$$[\![\boldsymbol{U}_k\boldsymbol{\gamma}_k^{MPE}]\!]=\frac{[\![\boldsymbol{U}_k\boldsymbol{\gamma}_k^{RRE}]\!]}{\sqrt{1-([\![\boldsymbol{U}_k\boldsymbol{\gamma}_k^{RRE}]\!]/[\![\boldsymbol{U}_{k-1}\boldsymbol{\gamma}_{k-1}^{RRE}]\!])^2}}\quad\text{when } \boldsymbol{s}_k^{MPE} \text{ exists.} \tag{3.29}$$

$$\frac{1}{[\![\boldsymbol{U}_k\boldsymbol{\gamma}_k^{RRE}]\!]^2}=\sum_{i\in S_k}\frac{1}{[\![\boldsymbol{U}_i\boldsymbol{\gamma}_i^{MPE}]\!]^2};\qquad S_k=\{0\le i\le k:\ \boldsymbol{s}_i^{MPE}\text{ exists}\}. \tag{3.30}$$

3.3 Implications of Theorems 3.1 and 3.2

Let us go back to the case in which $\{\boldsymbol{x}_m\}$ is generated as in $\boldsymbol{x}_{m+1}=\boldsymbol{f}(\boldsymbol{x}_m)$, $m=0,1,\ldots,$from the system $\boldsymbol{x}=\boldsymbol{f}(\boldsymbol{x})$. As we have already noted, with the residual associated with an arbitrary vector $\boldsymbol{x}$ defined as $\boldsymbol{r}(\boldsymbol{x})=\boldsymbol{f}(\boldsymbol{x})-\boldsymbol{x}$, (i) $\boldsymbol{U}_k\boldsymbol{\gamma}_k=\boldsymbol{r}(\boldsymbol{s}_k)$ when $\boldsymbol{f}(\boldsymbol{x})$ is linear, and (ii) $\boldsymbol{U}_k\boldsymbol{\gamma}_k\approx\boldsymbol{r}(\boldsymbol{s}_k)$ when $\boldsymbol{f}(\boldsymbol{x})$ is nonlinear and $\boldsymbol{s}_k$ is close to the solution $\boldsymbol{s}$ of $\boldsymbol{x}=\boldsymbol{f}(\boldsymbol{x})$. Then, Theorem 3.2 [especially (3.29)] implies that the convergence behaviors of MPE and RRE are interrelated in the following sense: MPE and RRE either converge well simultaneously or perform poorly simultaneously. Letting $\phi_k^{MPE}=[\![\boldsymbol{U}_k\boldsymbol{\gamma}_k^{MPE}]\!]$ and $\phi_k^{RRE}=[\![\boldsymbol{U}_k\boldsymbol{\gamma}_k^{RRE}]\!]$, and recalling that $\phi_k^{RRE}/\phi_{k-1}^{RRE}\le 1$ for all k, we have the following: (i) When $\phi_k^{RRE}/\phi_{k-1}^{RRE}$ is significantly smaller than 1, which means that RRE is performing well, ϕ_k^{MPE} is close to ϕ_k^{RRE}, that is, MPE is performing well too, and (ii) when ϕ_k^{MPE} is increasing, that is, MPE is performing poorly, $\phi_k^{RRE}/\phi_{k-1}^{RRE}$ is approaching 1, that is, RRE is performing poorly too. Thus, when the graph of ϕ_k^{MPE} has a peak for $\tilde{k}_1\le k\le\tilde{k}_2$, then the graph of ϕ_k^{RRE} has a plateau for $\tilde{k}_1\le k\le\tilde{k}_2$. This is known as the *peak-plateau* phenomenon in the context of Krylov subspace methods for linear systems.

4 Connection with Krylov subspace methods and concluding remarks

4.1 MPE and RRE on linear systems

Consider again the linear system of equations $\boldsymbol{x}=\boldsymbol{T}\boldsymbol{x}+\boldsymbol{d}$, where the matrix $(\boldsymbol{I}-\boldsymbol{T})$ is nonsingular, and generate $\{\boldsymbol{x}_m\}$ via $\boldsymbol{x}_{m+1}=\boldsymbol{T}\boldsymbol{x}_m+\boldsymbol{d}$, $m=0,1,\ldots,$with some initial vector $\boldsymbol{x}_0$. Apply MPE and RRE to $\{\boldsymbol{x}_m\}$ to obtain the vectors $\boldsymbol{s}_k$ as before. As already stated, $\boldsymbol{U}_k\boldsymbol{\gamma}_k = \boldsymbol{r}_k = \boldsymbol{r}(\boldsymbol{s}_k)$, where $\boldsymbol{r}(\boldsymbol{x}) = (\boldsymbol{T}\boldsymbol{x}+\boldsymbol{d}) - \boldsymbol{x}$ is the residual vector for the system $(\boldsymbol{I}-\boldsymbol{T})\boldsymbol{x} = \boldsymbol{d}$ associated with $\boldsymbol{x}$. In this case, we have the next theorem as a corollary of Theorems 3.1 and 3.2:

Theorem 4.1 *Let the sequence $\{\boldsymbol{x}_m\}$ be generated recursively via $\boldsymbol{x}_{m+1} = \boldsymbol{T}\boldsymbol{x}_m + \boldsymbol{d}$, $m = 0, 1, \dots,$the matrix $(\boldsymbol{I}-\boldsymbol{T})$ being nonsingular. Let also $\boldsymbol{r}(\boldsymbol{x}) = \boldsymbol{T}\boldsymbol{x}+\boldsymbol{d}-\boldsymbol{x}$ be the residual vector corresponding to $\boldsymbol{x}$. Let k_0 be the degree of the minimal polynomial of $\boldsymbol{T}$ with respect to $\boldsymbol{u}_0 = \boldsymbol{x}_1 - \boldsymbol{x}_0$. Then, for $k < k_0$, the vectors $\boldsymbol{s}_k^{MPE}$ and $\boldsymbol{s}_k^{RRE}$ obtained by applying MPE and RRE to $\{\boldsymbol{x}_m\}$ and their residual vectors $\boldsymbol{r}(\boldsymbol{s}_k^{MPE}) = \boldsymbol{r}_k^{MPE}$ and $\boldsymbol{r}(\boldsymbol{s}_k^{RRE}) = \boldsymbol{r}_k^{RRE}$ satisfy the following for this special case:*

1. *$\boldsymbol{s}_k^{RRE} = \boldsymbol{s}_{k-1}^{RRE}$ if and only if $\boldsymbol{s}_k^{MPE}$ fails to exist.*
2. *In case $\boldsymbol{s}_k^{MPE}$ exists, there hold*

$$\frac{1}{[\![\boldsymbol{r}_k^{RRE}]\!]^2} = \frac{1}{[\![\boldsymbol{r}_{k-1}^{RRE}]\!]^2} + \frac{1}{[\![\boldsymbol{r}_k^{MPE}]\!]^2}. \tag{4.1}$$

$$\frac{\boldsymbol{r}_k^{RRE}}{[\![\boldsymbol{r}_k^{RRE}]\!]^2} = \frac{\boldsymbol{r}_{k-1}^{RRE}}{[\![\boldsymbol{r}_{k-1}^{RRE}]\!]^2} + \frac{\boldsymbol{r}_k^{MPE}}{[\![\boldsymbol{r}_k^{MPE}]\!]^2}. \tag{4.2}$$

Consequently, we also have

$$\frac{\boldsymbol{s}_k^{RRE}}{[\![\boldsymbol{r}_k^{RRE}]\!]^2} = \frac{\boldsymbol{s}_{k-1}^{RRE}}{[\![\boldsymbol{r}_{k-1}^{RRE}]\!]^2} + \frac{\boldsymbol{s}_k^{MPE}}{[\![\boldsymbol{r}_k^{MPE}]\!]^2}. \tag{4.3}$$

In addition,

$$[\![\boldsymbol{r}_k^{RRE}]\!] < [\![\boldsymbol{r}_{k-1}^{RRE}]\!]. \tag{4.4}$$

3. *$\boldsymbol{s}_{k_0}^{MPE} = \boldsymbol{s}_{k_0}^{RRE} = \boldsymbol{s}$, where $\boldsymbol{s}$ is the solution to $(\boldsymbol{I}-\boldsymbol{T})\boldsymbol{x} = \boldsymbol{d}$.*

In view of (4.1), the results in (3.29) and (3.30) become

$$[\![\boldsymbol{r}_k^{MPE}]\!] = \frac{[\![\boldsymbol{r}_k^{RRE}]\!]}{\sqrt{1 - ([\![\boldsymbol{r}_k^{RRE}]\!]/[\![\boldsymbol{r}_{k-1}^{RRE}]\!])^2}} \quad \text{when } \boldsymbol{s}_k^{MPE} \text{ exists} \tag{4.5}$$

and

$$\frac{1}{[\![\boldsymbol{r}_k^{RRE}]\!]^2} = \sum_{i\in S_k} \frac{1}{[\![\boldsymbol{r}_i^{MPE}]\!]^2}; \quad S_k = \{0 \le i \le k :\ \boldsymbol{s}_i^{MPE} \text{ exists}\}. \tag{4.6}$$

4.2 Equivalence of redefined MPE and RRE to Krylov subspace methods for linear systems

Theorem 2.4 in [24] concerns the mathematical equivalence of vector extrapolation methods to Krylov subspace methods, when all these methods are defined using the standard Euclidean inner product $(\cdot\,,\cdot)$ and the standard norm $\|\cdot\|$ induced by $(\cdot\,,\cdot)$: This theorem states specifically that MPE and RRE are equivalent to, respectively, the full orthogonalization method (FOM) of Arnoldi and the method of generalized minimal residuals (GMR) when

- MPE and RRE are being applied to the sequence $\{\boldsymbol{x}_m\}$ obtained via $\boldsymbol{x}_{m+1} = \boldsymbol{T}\boldsymbol{x}_m + \boldsymbol{d}$, $m = 0, 1, \dots,$with some $\boldsymbol{x}_0$, and

- FOM and GMR are being applied to $(\boldsymbol{I}-\boldsymbol{T})\boldsymbol{x}=\boldsymbol{d}$, starting with the same initial vector $\boldsymbol{x}_0$.

As stated in Theorem 4.2 below, this theorem holds true also when MPE, RRE, FOM, and GMR are defined using the weighted inner product $\langle\cdot\,,\cdot\rangle$ and the weighted norm $[\![\cdot]\!]$ induced by $\langle\cdot\,,\cdot\rangle$. In the next paragraph, we state these definitions of FOM and GMR.

For a nonsingular linear system $\boldsymbol{A}\boldsymbol{x}=\boldsymbol{b}$, whose solution we denote by $\boldsymbol{s}$, FOM and GMR construct their approximations $\boldsymbol{w}_k$ to $\boldsymbol{s}$ as follows: Define the residual vector corresponding to $\boldsymbol{x}$ by $\boldsymbol{r}(\boldsymbol{x})=\boldsymbol{b}-\boldsymbol{A}\boldsymbol{x}$ and denote $\boldsymbol{r}_0=\boldsymbol{r}(\boldsymbol{x}_0)$ for some initial vector $\boldsymbol{x}_0$. Let $\mathcal{K}_k(\boldsymbol{A};\boldsymbol{r}_0)=\text{span}\{\boldsymbol{r}_0,\boldsymbol{A}\boldsymbol{r}_0,\ldots,\boldsymbol{A}^{k-1}\boldsymbol{r}_0\}$. Then, for each method, the approximation $\boldsymbol{w}_k$ to $\boldsymbol{s}$ is of the form $\boldsymbol{w}_k=\boldsymbol{x}_0+\boldsymbol{y}$ such that $\boldsymbol{y}\in\mathcal{K}_k(\boldsymbol{A};\boldsymbol{r}_0)$, and $\boldsymbol{y}$ is the vector to be determined. Using the weighted inner product $\langle\cdot\,,\cdot\rangle$ and the norm $[\![\cdot]\!]$ induced by it, these methods can be redefined as follows:

- For FOM, $\boldsymbol{y}$ is determined by requiring that $\langle\boldsymbol{z},\boldsymbol{r}_k^{\text{FOM}}\rangle=0$ for all $\boldsymbol{z}\in\mathcal{K}_k(\boldsymbol{A};\boldsymbol{r}_0)$, where $\boldsymbol{r}_k^{\text{FOM}}=\boldsymbol{r}(\boldsymbol{w}_k^{\text{FOM}})$.
- For GMR, $\boldsymbol{y}$ is determined by requiring that $[\![\boldsymbol{r}_k^{\text{GMR}}]\!]=\min_{\boldsymbol{y}\in\mathcal{K}_k(\boldsymbol{A};\boldsymbol{r}_0)}[\![\boldsymbol{r}(\boldsymbol{x}_0+\boldsymbol{y})]\!]$, where $\boldsymbol{r}_k^{\text{GMR}}=\boldsymbol{r}(\boldsymbol{w}_k^{\text{GMR}})$.

Then we have the following generalization of Theorem 2.4 in [24]:

Theorem 4.2 *Consider the nonsingular linear system $(\boldsymbol{I}-\boldsymbol{T})\boldsymbol{x}=\boldsymbol{d}$. Apply FOM and GMR to this system starting with some initial vector $\boldsymbol{x}_0$. Apply MPE and RRE to the sequence $\{\boldsymbol{x}_m\}$ obtained from $\boldsymbol{x}_{m+1}=\boldsymbol{T}\boldsymbol{x}_m+\boldsymbol{d}$, $m=0,1,\ldots,$with the same initial vector $\boldsymbol{x}_0$. Then*

$$\boldsymbol{w}_k^{\text{FOM}}=\boldsymbol{s}_k^{\text{MPE}}\quad\textit{and}\quad\boldsymbol{w}_k^{\text{GMR}}=\boldsymbol{s}_k^{\text{RRE}},\tag{4.7}$$

when all four methods are defined using the same weighted inner product $\langle\cdot\,,\cdot\rangle$ and the norm $[\![\cdot]\!]$ induced by it. Consequently, all of the results of Theorem 4.1 apply verbatim to the vectors $\boldsymbol{w}_k^{\text{FOM}}$ and $\boldsymbol{w}_k^{\text{GMR}}$.

Proof The same as that of [24, Theorem 2.4]. □

In view of Theorem 4.2, Theorem 4.1 holds verbatim with $\boldsymbol{s}_k^{\text{MPE}}$, $\boldsymbol{r}_k^{\text{MPE}}$ and $\boldsymbol{s}_k^{\text{RRE}}$, $\boldsymbol{r}_k^{\text{RRE}}$ there replaced by $\boldsymbol{w}_k^{\text{FOM}}$, $\boldsymbol{r}_k^{\text{FOM}}$ and $\boldsymbol{w}_k^{\text{GMR}}$, $\boldsymbol{r}_k^{\text{GMR}}$, respectively. Of course, these results for FOM and GMR are not new. As already mentioned, they were given originally by Weiss [35] and by Brown [4], and developed further in the papers mentioned in Section 1.

Note that the vectors $\boldsymbol{w}_k^{\text{FOM}}$ and $\boldsymbol{w}_k^{\text{GMR}}$ can be obtained numerically by modifying the known algorithms for FOM and GMR such that the Euclidean inner product and the associated norm are replaced by a weighted inner product and the associated norm. This is precisely what is done in the paper by Essai [10], which was mentioned in Section 1.

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