Minimal Polynomial and Reduced Rank Extrapolation Methods Are Related

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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 \( \{x_m\} \). 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 \( s_k \) to the limit or antilimit of \( \{x_m\} \) that are of the form \( s_k = \sum_{i=0}^{k} \gamma_i x_i \) with \( \sum_{i=0}^{k} \gamma_i = 1 \), for some scalars \( \gamma_i \). 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 \( s_k^{\text{MPE}} \) and \( s_k^{\text{RRE}} \) produced by the two methods are related in more than one way, and independently of the way the \( x_m \) are generated. One of our results states that RRE stagnates, in the sense that \( s_k^{\text{RRE}} = s_{k-1}^{\text{RRE}} \), if and only if \( s_k^{\text{MPE}} \) does not exist. Another result states that, when \( s_k^{\text{MPE}} \) exists, there holds

\[
\mu_k s_k^{\text{RRE}} = \mu_{k-1} s_{k-1}^{\text{RRE}} + \nu_k s_k^{\text{MPE}} \quad \text{with} \quad \mu_k = \mu_{k-1} + \nu_k,
\]

for some positive scalars \( \mu_k, \mu_{k-1}, \) and \( \nu_k \) that depend only on \( s_k^{\text{RRE}}, s_{k-1}^{\text{RRE}}, \) and \( s_k^{\text{MPE}} \), 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.

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1 Introduction

Minimal Polynomial Extrapolation (MPE) of Cabay and Jackson [5] and Reduced Rank Extrapolation (RRE) of Kaniel and Stein [15], Eddy [6], and Meˇ sina [16] are two polynomial methods of convergence acceleration for sequences of vectors. 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 [28] and, more recently, by Sidi [24]. Their convergence and stability properties were analyzed in the papers by Sidi [20], [23], Sidi and Bridger [25], and Sidi and Shapira [26], [27]. Their connection with known Krylov subspace methods for the solution of linear systems of equations was explored in Sidi [21]. In Ford and Sidi [9], 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 [22]. 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 very closely related in more than one way. A partial description of the results of this investigation are given in the next paragraph.

Let \( \{x_m\} \) be an arbitrary sequence of vectors in \( \mathbb{C}^N \) endowed with a general (not necessarily standard Euclidean) inner product and the norm induced by it, and let \( s^\text{MPE}_k \) and \( s^\text{RRE}_k \) be the vectors (approximations to \( \lim_{m \to \infty} x_m \), for example) produced by MPE and RRE from the \( k+2 \) vectors \( x_0, x_1, \ldots, x_{k+1} \). It is known that \( s^\text{RRE}_k \) always exists, but \( s^\text{MPE}_k \) may not always exist. One of our results states that, RRE stagnates, in the sense that

\[
s^\text{RRE}_k = s^\text{RRE}_{k-1} \iff s^\text{MPE}_k \text{ does not exist}. \tag{1.1}
\]

Another result states that, when \( s^\text{MPE}_k \) exists, there holds

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

for some positive scalars \( \mu_k, \mu_{k-1}, \) and \( \nu_k \) that depend only on \( s^\text{RRE}_k, s^\text{RRE}_{k-1}, \) and \( s^\text{MPE}_k \), respectively. The precise results and the conditions under which they hold will be given in the next sections.

When the sequence \( \{x_m\} \) is generated from a linear nonsingular system of equations \( x = T x + d \) via the fixed-point iterative scheme \( x_{m+1} = T x_m + d \), the vectors \( s^\text{MPE}_k \) and \( s^\text{RRE}_k \) 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

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1The formulations of RRE given in Kaniel and Stein [15] and Meˇ sina [16] are essentially the same, but they are entirely different from that in Eddy [6]. The mathematical equivalence of the different formulations is shown in Smith, Ford, and Sidi in [28].

2Throughout this work, we will use boldface lowercase letters to denote column vectors. In particular, we will denote the zero column vector by \( 0 \). Similarly, we will use boldface upper case letters to denote matrices.
the linear system \((I - T)x = d\), starting with \(x_0\) 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 \textit{Arnoldi–Gram–Schmidt process}, for computing an orthonormal basis for a Krylov subspace. For a discussion of FOM and more, see also Saad \[17\]. Different algorithms were given for GMR by Axelsson \[2\], by Young and Jea \[33\], by Eisenstat, Elman, and Schultz \[8\], known as \textit{Generalized Conjugate Residuals} (GCR), and by Saad and Schultz \[19\], 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 \[10\], Saad \[18\], and van der Vorst \[29\].

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 \[31\] originally. This topic has been analyzed further in the papers by Gutknecht \[13, 14\], Weiss \[32\], Zhou and Walker \[34\], Walker \[30\], and Eiermann and Ernst \[7\], 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 \(\{x_m\}\) is \textit{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 \[31\] in the presence of such \(\{x_m\}\). 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 FOM and RRE apply to linear systems only. Actually, our results apply to \textit{arbitrary} sequences \(\{x_m\}\), 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 \(\{x_m\}\) 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 \textit{arbitrary} sequences \(\{x_m\}\), 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 \textit{unified} algorithm for their implementation, thus also providing the theoretical background necessary for the rest of this work.

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 \(\{x_m\}\) generated from a linear nonsingular system of equations via fixed-point iterative schemes, and show that

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\(^3\)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 \[22\] still use the standard Euclidean inner product and the norm induced by it, however.
our main results reduce to the known analogous results of [4] and [31] 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

$$\langle y, z \rangle = y^* M z \quad \text{and} \quad \|z\| = \sqrt{\langle z, z \rangle} = \sqrt{z^* M z},$$

(1.3)

where $M \in \mathbb{C}^{N \times N}$ is a hermitian positive definite matrix.

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

$$(y, z) = y^* z \quad \text{and} \quad \|z\| = \sqrt{z^* z}.$$ (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 originally in the papers by Gulliksson and Wedin [12] and Gulliksson [11]. It turns out to be the most natural extension of the ordinary QR factorization when orthogonality of two vectors $y, z \in \mathbb{C}^N$ is in the sense $\langle y, z \rangle = 0$. For convenience, and to make this work self-contained, we discuss it briefly in the appendix. For much more, we refer the reader to [12] and [11].

2 MPE and RRE redefined using a weighted inner product

2.1 General preliminaries

Let $\{x_m\}$ 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

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

(2.1)

that is, from

$$x_{m+1} = f(x_m), \quad m = 0, 1, \ldots,$$ (2.2)

$x_0$ being an initial vector chosen by the user. Normally, $N$ is large and $f(x)$ is a sparse vector-valued function. Now, when the sequence $\{x_m\}$ converges, it does so to the solution $s$, that is, $\lim_{m \to \infty} x_m = s$. In case $\{x_m\}$ diverges, we call $s$ the antilimit of $\{x_m\}$; vector extrapolation methods in general, and MPE and RRE in particular, may produce sequences of approximations that converge to $s$, the antilimit of $\{x_m\}$, in such a case.

Let us define the vectors $u_i$ via

$$u_i = x_{i+1} - x_i, \quad i = 0, 1, \ldots,$$ (2.3)

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

$$U_k = \begin{bmatrix} u_0 & u_1 & \cdots & u_k \end{bmatrix}, \quad k = 0, 1, \ldots. \quad (2.4)$$

Of course, there is an integer $k_0 \leq N$, such that the matrices $U_k$, $k = 0, 1, \ldots, k_0 - 1$, are of full rank, but $U_{k_0}$ is not; that is,

$$\text{rank}(U_k) = k + 1, \quad k = 0, 1, \ldots, k_0 - 1; \quad \text{rank}(U_{k_0}) = k_0. \quad (2.5)$$

(Of course, this is the same as saying that $\{u_0, u_1, \ldots, u_{k_0-1}\}$ is a linearly independent set, but $\{u_0, u_1, \ldots, u_{k_0}\}$ is not.)

Then, both MPE and RRE produce approximations $s_k$ (with $k \leq k_0$) to the solution $s$ of (2.1) that are of the form

$$s_k = \sum_{i=0}^{k} \gamma_i x_i; \quad \sum_{i=0}^{k} \gamma_i = 1, \quad (2.6)$$

for some scalars $\gamma_i$. On account of the condition $\sum_{i=0}^{k} \gamma_i = 1$, and because $x_i = x_0 + \sum_{j=0}^{i-1} u_j$, we can rewrite (2.6) in the form

$$s_k = x_0 + \sum_{j=0}^{k-1} \xi_j u_j; \quad \xi_j = \sum_{i=0}^{k-1} \gamma_i, \quad j = 0, 1, \ldots, k - 1, \quad (2.7)$$

which can also be expressed in matrix terms as in

$$s_k = x_0 + U_{k-1} \xi, \quad \xi = [\xi_0, \xi_1, \ldots, \xi_{k-1}]^T. \quad (2.8)$$

We will make use of both representations of $s_k$, namely, (2.6) and (2.7)–(2.8), later. The $\gamma_i$ and $\xi_j$ for MPE are, of course, different from those for RRE, in general.

In the sequel, where confusion may arise, we will denote the vectors $s_k$ resulting from MPE and RRE by $s_k^{\text{MPE}}$ and $s_k^{\text{RRE}}$, respectively. Similarly, to avoid confusion, we will denote the vectors $\gamma = [\gamma_0, \gamma_1, \ldots, \gamma_k]^T$ and $\xi = [\xi_0, \xi_1, \ldots, \xi_{k-1}]^T$ corresponding to $s_k$ by $\gamma_k^{\text{MPE}}$ or $\gamma_k^{\text{RRE}}$ and $\xi_k^{\text{MPE}}$ or $\xi_k^{\text{RRE}}$, respectively, depending on the context.

We now describe how the $\gamma_i$ 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 $\gamma_i$ for MPE and RRE

#### 2.2.1 The $\gamma_i$ for MPE

Solve by least squares the linear overdetermined system of equations

$$\sum_{i=0}^{k-1} c_i u_i = -u_k \quad (2.9)$$

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

$$U_{k-1} c' = -u_k; \quad c' = [c_0, c_1, \ldots, c_{k-1}]^T. \quad (2.10)$$
and the least squares problem becomes

$$\min_{c'} [U_{k-1}c' + u_k].$$

(2.11)

Since $U_{k-1}$ has full column rank, this problem has a unique solution for $c'$. Next, let $c_k = 1$, and compute

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

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

2.2.2 The $\gamma_i$ for RRE

Solve by least squares the linear overdetermined system of equations

$$\sum_{i=0}^{k} \gamma_i u_i = 0, \quad (2.13)$$

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

$$U_k \gamma = 0, \quad \gamma = [\gamma_0, \gamma_1, \ldots, \gamma_k]^T, \quad (2.14)$$

and the constrained least squares problem becomes

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

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

2.3 The special case $k = k_0$

With $s_k$ for MPE and RRE already defined, we start with a discussion of the case in which $k = k_0$.

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

1. Provided $s_{k_0}^{\text{MPE}}$ exists, we have $s_{k_0}^{\text{MPE}} = s_{k_0}^{\text{RRE}}$.

2. Assume the sequence $\{x_m\}$ is generated via (2.1) and (2.2) with a linear $f(x)$, namely, with $f(x) = T x + d$, where $T \in \mathbb{C}^{N \times N}$ is some constant matrix and $d \in \mathbb{C}^N$ is some constant vector, and $(I - T)$ is nonsingular. Then $s_{k_0}^{\text{MPE}}$ exists, and there holds $s_{k_0}^{\text{MPE}} = s_{k_0}^{\text{RRE}} = s$, $s$ being the (unique) solution to $x = T x + d$. In this case, $k_0$ is the degree of the minimal polynomial of $T$ with respect to the vector $u_0$. 

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Proof. We start by observing that the matrix $U_{k_0-1}$ has full rank and that the vector $u_{k_0}$ is a linear combination of $u_0, u_1, \ldots, u_{k_0-1}$. As result, the linear system in (2.10) is consistent, hence has a unique solution for $c'$ in the regular sense, this solution being also the solution to the minimization problem in (2.11). Letting $c_k = 1$ and proceeding as in (2.12), we obtain the $\gamma_{MPE}^k$. A similar argument based on (2.14) and (2.15) shows that $\gamma_{RRE}^k = \gamma_{MPE}^k$. This proves part 1 of the theorem. Part 2 can be proved as in [28], for example.

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

2.4 Determination of the $\gamma_i$ via weighted QR factorization

A numerically stable and computationally economical algorithm for computing the $\gamma_i$ for both MPE and RRE when $M = I$ has been given in Sidi [22]. A nice feature of this algorithm is that it proceeds via the QR factorization of the matrices $U_k$ 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 [22] can be formulated for this case. This can be accomplished by proceeding via the weighted QR factorization of $U_k$. Even though this algorithm, just as that in [22], 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 [22].

We start with the weighted QR factorization of $U_k$. For convenience, we describe this topic in some detail in the appendix. Since $U_k$ is of full column rank, by Theorem A.1 in the appendix, it has a unique weighted QR factorization given as in

$$U_k = Q_k R_k; \quad Q_k \in \mathbb{C}^{N \times (k+1)}, \quad R_k \in \mathbb{C}^{(k+1) \times (k+1)},$$

(2.16)

where $Q_k$ is unitary in the sense that $Q_k^* M Q_k = I_{k+1}$ since $k < N$, and $R_k$ is upper triangular with positive diagonal elements; that is,

$$Q_k = [q_0 \mid q_1 \mid \cdots \mid q_k], \quad R_k = \begin{bmatrix} r_{00} & r_{01} & \cdots & r_{0k} \\ r_{11} & \cdots & r_{1k} \\ \vdots & \ddots & \vdots \\ r_{kk} & & & \end{bmatrix},$$

(2.17)

$$q_i^* M q_j = \delta_{ij} \quad \forall \ i, j; \quad r_{ij} = q_i^* M u_j \quad \forall \ i \leq j; \quad r_{ii} > 0 \quad \forall \ i.$$  \hspace{1cm} (2.18)

(Note that, having positive diagonal elements and being upper triangular, $R_k$ is also nonsingular.) Clearly, just as $U_k$ has the partitioning $U_k = [U_{k-1} \mid u_k]$, $Q_k$ and $R_k$ have the partitionings

$$Q_k = [Q_{k-1} \mid q_k] \quad \text{and} \quad R_k = \begin{bmatrix} R_{k-1} \\ 0^T \end{bmatrix}, \quad \rho_k = [r_{0k}, r_{1k}, \ldots, r_{k-1,k}]^T.$$ \hspace{1cm} (2.19)

We will make use of the following easily verifiable lemma in the sequel:
Lemma 2.2 Let \( P \in \mathbb{C}^{N \times j} \) and \( P^*MP = I_j \).

Then \( \langle Py, Pz \rangle = y^*z = (y, z) \) and \( \|Pz\| = \sqrt{z^*z} = \|z\| \).

By this lemma, for arbitrary \( k \), we have \( \langle Q_ky, Q_kz \rangle = y^*z = (y, z) \) and \( \|Q_kz\| = \sqrt{z^*z} = \|z\| \) \quad (2.20)

and \( \|U_kz\| = \|R_kz\| \). \quad (2.21)

Of these, (2.20) follows from \( Q_k^*M Q_k = I_{k+1} \), while (2.21) follows from \( U_k = Q_k R_k \) and (2.20).

2.4.1 Determination of \( \gamma_k \) for MPE

Let us fix \( c_k = 1 \) and let \( c = [c_0, c_1, \ldots, c_k]^T = \left[ \frac{c'}{1} \right] \). Then we have

\[ U_{k-1}c' + u_k = U_k c \quad \Rightarrow \quad \|U_{k-1}c' + u_k\| = \|U_k c\| = \|R_k c\|, \]

and the minimization problem in (2.11) becomes,

\[ \min_{c'} \|R_k c\|. \]

By (2.19),

\[ R_k c = \begin{bmatrix} R_{k-1} & \rho_k \\ 0^T \end{bmatrix} \begin{bmatrix} c' \\ 1 \end{bmatrix} = \begin{bmatrix} R_{k-1}c' + \rho_k \\ r_{kk} \end{bmatrix}, \]

which, upon taking norms, yields

\[ \|R_k c\|^2 = \|R_{k-1}c' + \rho_k\|^2 + r_{kk}^2. \]

Clearly, by the fact that \( R_{k-1} \) is a nonsingular \( k \times k \) matrix, the minimum of \( \|R_k c\| \) with respect to \( c' \) is achieved when \( c' \) satisfies

\[ R_{k-1}c' + \rho_k = 0 \quad \Rightarrow \quad R_{k-1}c' = -\rho_k \quad \Rightarrow \quad c' = -R_{k-1}^{-1}\rho_k. \]

Of course, \( c' \) is unique, and so is \( c \).

With \( c' = -R_{k-1}^{-1}\rho_k \), the vector \( \gamma_k \) in MPE is obtained as in

\[ \gamma_k^{\text{MPE}} = \frac{c}{\hat{e}_k^T c}, \quad c = \left[ \begin{array}{c} c' \\ 1 \end{array} \right]. \]

Of course, this is valid only when \( \hat{e}_k^T c = \sum_{i=0}^k c_i \neq 0 \), hence only when \( s_k^{\text{MPE}} \) exists.

The vector \( c \) exists uniquely whether \( s_k^{\text{MPE}} \) exists or not, however.
2.4.2 Determination of $\gamma_k$ for RRE

By the fact that $[U_k y] = ||R_k y||$, the minimization problem in \ref{eq:2.15} becomes

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

and equivalently,

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

By the lemma in \cite[Appendix A]{22}, the solution for the vector $\gamma_k$ in RRE proceeds through the following steps:

\begin{equation}
R_k^* R_k h = \hat{e}_k, \quad h = [h_0, h_1, \ldots, h_k]^T \quad (\text{solve for } h). \tag{2.25}
\end{equation}

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

\begin{equation}
\gamma_k^{\text{RRE}} = \lambda h. \tag{2.27}
\end{equation}

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

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

\begin{equation}
\lambda = \frac{1}{\hat{e}_k^T (R_k^* R_k)^{-1} \hat{e}_k} = \frac{1}{||R_k^* \hat{e}_k||^2} \tag{2.28}
\end{equation}

and

\begin{equation}
\gamma_k^{\text{RRE}} = \frac{(R_k^* R_k)^{-1} \hat{e}_k}{\hat{e}_k^T (R_k^* R_k)^{-1} \hat{e}_k} = \frac{R_k^{-1}(R_k^{*-1}\hat{e}_k)}{||R_k^{*-1}\hat{e}_k||^2}. \tag{2.29}
\end{equation}

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

2.5 Unified algorithm for MPE and RRE

Once the $\gamma_k$ have been computed as described above, the computation of $s_k$ can be achieved via \ref{eq:2.7}--\ref{eq:2.8} as follows: First, we compute the vector $\xi_k = [\xi_0, \xi_1, \ldots, \xi_k]^T$ via \ref{eq:2.7}, and then, by invoking $U_{k-1} = Q_{k-1} R_{k-1}$, we compute $s_k$ via \ref{eq:2.8}, as in

\begin{equation}
s_k = x_0 + Q_{k-1}(R_{k-1}\xi_k) = x_0 + \sum_{j=0}^{k-1} \eta_j u_j; \tag{2.30}
\end{equation}

\begin{equation}
\eta = R_{k-1}\xi_k, \quad \eta = [\eta_0, \eta_1, \ldots, \eta_{k-1}]^T. \tag{2.30}
\end{equation}

For convenience, we give a complete description of the unified algorithm in Table 2.1.
Table 2.1: Unified algorithm for implementing MPE and RRE.

Step 0. Input: The hermitian positive definite matrix $M \in \mathbb{C}^{N \times N}$, the integer $k$, and the vectors $x_0, x_1, \ldots, x_{k+1}$.

Step 1. Compute $u_i = \Delta x_i = x_{i+1} - x_i$, $i = 0, 1, \ldots, k$.

Set $U_j = [u_0 | u_1 | \cdots | u_j] \in \mathbb{C}^{N \times (j+1)}$, $j = 0, 1, \ldots$.

Compute the weighted QR factorization of $U_k$, namely, $U_k = Q_k R_k$; $Q_k = [q_0 | q_1 | \cdots | q_k]$ unitary in the sense $Q_k^* M Q_k = I_{k+1}$, and $R_k = [r_{ij}]_{0 \leq i,j \leq k}$ upper triangular, $r_{ij} = q_i^* M u_j$.

$(U_{k-1} = Q_{k-1} R_{k-1}$ is contained in $U_k = Q_k R_k.)$

Step 2. Computation of $\gamma_k = [\gamma_0, \gamma_1, \ldots, \gamma_k]^T$:

For MPE:

Solve the (upper triangular) linear system

$$R_{k-1} c' = -\rho_k; \quad \rho_k = [r_{0k}, r_{1k}, \ldots, r_{k-1,k}]^T, \quad c' = [c_0, c_1, \ldots, c_{k-1}]^T.$$

(Note that $\rho_k = Q_{k-1}^* M u_k$.)

Set $c_k = 1$ and compute $\alpha = \sum_{i=0}^k c_i$.

Set $\gamma_k = c/\alpha$; that is, $\gamma_i = c_i/\alpha$, $i = 0, 1, \ldots, k$, provided $\alpha \neq 0$.

For RRE:

Solve the linear system

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

(This amounts to solving two triangular (lower and upper) systems.)

Set $\lambda = (\sum_{i=0}^k h_i)^{-1}$. (Note that $\lambda$ is real and positive.)

Set $\gamma_k = \lambda h_i$; that is, $\gamma_i = \lambda h_i$, $i = 0, 1, \ldots, k$.

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

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

Compute $s_k^{MPE}$ and $s_k^{RRE}$ via

$$s_k = x_0 + Q_{k-1}(R_{k-1} \xi_k) = x_0 + Q_{k-1} \eta.$$

[For this, first compute $\eta = R_{k-1} \xi_k$, $\eta = [\eta_0, \eta_1, \ldots, \eta_{k-1}]^T$.

Next, set $s_k = x_0 + \sum_{i=0}^{k-1} \eta_i q_i$.]

9
2.6 Error assessment

Let us now return to the system of equations in (2.1). If $x$ is an approximation to the solution $s$ of this system, then one good measure of the accuracy of $x$ is (some norm of) the residual vector $r(x)$ corresponding to $x$ that is given by

$$r(x) = f(x) - x.$$ \hspace{0.5cm} (2.31)

This is natural because $\lim_{x \to s} r(x) = r(s) = 0$. In case the sequence $\{x_m\}$ is being generated as in (2.2) for solving (2.1), our measure for the quality of $s_k$ will then be $U_k\gamma_k$. The following have been shown in [22]:

- When $f(x)$ is linear [that is, $f(x) = T x + d$ for some constant matrix $T \in \mathbb{C}^{N \times N}$ and constant vector $d \in \mathbb{C}^N$], $r(s_k) = U_k\gamma_k$ exactly.

- When $f(x)$ is nonlinear, $U_k\gamma_k$ serves as an approximation to $r(s_k)$, that is, $r(s_k) \approx U_k\gamma_k$, and $U_k\gamma_k$ gets closer and closer to $r(s_k)$ as convergence is approached.

In addition, $\left[U_k\gamma_k\right]$, the weighted norm of $U_k\gamma_k$, can be obtained, without actually computing $U_k\gamma_k$ 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 $U_k\gamma_k^{\text{MPE}}$ and $U_k\gamma_k^{\text{RRE}}$ satisfy

$$\left[U_k\gamma_k^{\text{MPE}}\right] = r_{kk}\gamma_k \quad \text{and} \quad \left[U_k\gamma_k^{\text{RRE}}\right] = \sqrt{\lambda}. \hspace{0.5cm} (2.32)$$

**Remarks.**

1. Of course, $\gamma_k$ in (2.32) is the last component of $\gamma_k^{\text{MPE}}$ corresponding to $s_k^{\text{MPE}}$. Similarly, $\lambda$ in (2.32) is as defined in (2.26) for $s_k^{\text{RRE}}$.

2. Clearly, (2.32) is valid for all sequences $\{x_m\}$, whether these are generated by a (linear or nonlinear) fixed-point iterative scheme or otherwise.

**Proof.** By (2.21), we have that $\left[U_k\gamma_k\right] = \|R_k\gamma_k\|$. Therefore, it is enough to look at $\|R_k\gamma_k^{\text{MPE}}\|$ and $\|R_k\gamma_k^{\text{RRE}}\|$.

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

$$R_k\gamma_k^{\text{MPE}} = \frac{1}{\hat{e}_k^Tc} (R_kc) = \gamma_k \begin{bmatrix} 0 \\ r_{kk} \end{bmatrix} = r_{kk}\gamma_k \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$ 

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

As for RRE, by (2.29), we have

$$R_k\gamma_k^{\text{RRE}} = \frac{R_k^{-}\hat{e}_k}{\|R_k^{-}\hat{e}_k\|^2}.$$ 

Taking norms on both sides, and invoking (2.28), we obtain the result for RRE. \[\blacksquare\]
3 MPE and RRE are related

We begin by restating that since

\[ U_k \gamma_k = Q_k (R_k \gamma_k) \quad \text{and} \quad \|U_k \gamma_k\| = \|R_k \gamma_k\|, \tag{3.1} \]

and since \( Q_k \) and \( R_k \) are the same for both MPE and RRE, the vector that is of relevance for both methods is \( R_k \gamma_k \), and we turn to the study of this vector. In addition, we express everything in terms of the vectors \( c' \) and \( c \) and the matrices \( Q_k \) and \( R_k \), which do not depend either on \( s_{MPE}^k \) or \( s_{RRE}^k \). In the developments that follow, we will also recall that \( \|y\| = \sqrt{y^*y} \) always.

3.1 \( R_k \gamma_k \) for MPE and RRE and an identity

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

\[ R_k \gamma_{\text{MPE}}^k = \frac{1}{\hat{e}_k^T c} R_k c, \]

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

\[ R_k \gamma_{\text{MPE}}^k = \frac{r_{kk}}{\hat{e}_k^T c} \begin{bmatrix} 0 \\ 1 \end{bmatrix}. \tag{3.2} \]

Of course, this immediately implies that

\[ \|R_k \gamma_{\text{MPE}}^k\| = \frac{r_{kk}}{|\hat{e}_k^T c|}. \tag{3.3} \]

As for RRE, by (2.29), we have

\[ R_k \gamma_{\text{RRE}}^k = \frac{R_{k^-}^* \hat{e}_k}{\|R_{k^-}^* \hat{e}_k\|^2}. \tag{3.4} \]

Of course, this immediately implies that

\[ \|R_k \gamma_{\text{RRE}}^k\| = \frac{1}{\|R_{k^-}^* \hat{e}_k\|} \quad \Rightarrow \quad R_{k^-}^* \hat{e}_k = \frac{R_k \gamma_{\text{RRE}}^k}{\|R_{k^-}^* \hat{e}_k\|^2}. \tag{3.5} \]

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

\[ R_k^{-1} = \begin{bmatrix} R_k^{-1} & c'/r_{kk} \\ 0^T & 1/r_{kk} \end{bmatrix} \quad \Rightarrow \quad R_k^{-*} = \begin{bmatrix} R_k^{-*} & 0 \\ c'/r_{kk} & 1/r_{kk} \end{bmatrix}. \tag{3.6} \]

Consequently, invoking also \( \hat{e}_k = \begin{bmatrix} \hat{e}_{k-1} \\ 1 \end{bmatrix} \), we have

\[ R_{k^-}^* \hat{e}_k = \begin{bmatrix} R_{k-1}^{-*} & 0 \\ c'/r_{kk} & 1/r_{kk} \end{bmatrix} \begin{bmatrix} \hat{e}_{k-1} \\ 1 \end{bmatrix} = \begin{bmatrix} R_{k-1}^{-*} \hat{e}_{k-1} \\ c' \hat{e}_{k-1}/r_{kk} + 1/r_{kk} \end{bmatrix} = \begin{bmatrix} R_{k-1}^{-*} \hat{e}_{k-1} \\ \hat{e}_k^T c/r_{kk} \end{bmatrix}. \tag{3.7} \]
which, by (3.5), can also be expressed as in
\[ \frac{1}{\| R_k \gamma_k^{\text{RRE}} \|^2} R_k \gamma_k^{\text{RRE}} = \frac{1}{\| R_{k-1} \gamma_{k-1}^{\text{RRE}} \|^2} \left[ \frac{R_{k-1} \gamma_{k-1}^{\text{RRE}}}{0} \right] + \frac{\bar{e}_k^T c}{r_{kk}} \begin{bmatrix} 0 \\ 1 \end{bmatrix}. \] (3.8)

Clearly, (3.8) is an identity for RRE relating \( s_{RRE}^{k-1} \) and \( s_{RRE}^k \); 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 vector \( c \) exists uniquely for all \( k < k_0 \). Thus, (3.8) is valid whether \( s_{MPE}^k \) exists or not.

### 3.2 Main results

The following theorem is our first main result, and concerns the case in which \( s_{MPE}^k \) does not exist and RRE stagnates.

**Theorem 3.1** 1. In case \( s_{MPE}^k \) does not exist, there holds
\[ U_k \gamma_k^{\text{RRE}} = U_{k-1} \gamma_{k-1}^{\text{RRE}}. \] (3.9)
Consequently, we also have that
\[ s_k^{\text{RRE}} = s_{k-1}^{\text{RRE}}. \] (3.10)

2. Conversely, if (3.10) holds, then \( s_{MPE}^k \) does not exist.

**Proof.** The proof is based on the fact that \( s_{MPE}^k \) exists if and only if \( e_k^T c \neq 0 \).

**Proof of part 1:** Since \( e_k^T c = 0 \) when \( s_{MPE}^k \) does not exist, by (3.8),
\[ \frac{1}{\| R_k \gamma_k^{\text{RRE}} \|^2} R_k \gamma_k^{\text{RRE}} = \frac{1}{\| R_{k-1} \gamma_{k-1}^{\text{RRE}} \|^2} \left[ \frac{R_{k-1} \gamma_{k-1}^{\text{RRE}}}{0} \right]. \] (3.11)

Taking norms in (3.11), we obtain
\[ \| R_k \gamma_k^{\text{RRE}} \| = \| R_{k-1} \gamma_{k-1}^{\text{RRE}} \| \Rightarrow R_k \gamma_k^{\text{RRE}} = \left[ \frac{R_{k-1} \gamma_{k-1}^{\text{RRE}}}{0} \right]. \] (3.12)

Multiplying both sides of (3.12) on the left by \( Q_k \), we have
\[ U_k \gamma_k^{\text{RRE}} = Q_k (R_k \gamma_k^{\text{RRE}}) = \left[ Q_{k-1} | q_k \right] \left[ \frac{R_{k-1} \gamma_{k-1}^{\text{RRE}}}{0} \right] \]
\[ = Q_{k-1} (R_{k-1} \gamma_{k-1}^{\text{RRE}}) = U_{k-1} \gamma_{k-1}^{\text{RRE}}. \] (3.13)

Thus, we have proved the result in (3.9).

**Rewriting (3.13) in the form**
\[ U_k \gamma_k^{\text{RRE}} = U_k \left[ \frac{\gamma_{k-1}^{\text{RRE}}}{0} \right], \] (3.14)
and invoking the fact that $U_k$ is of full column rank, we obtain

$$\gamma^{\text{RRE}}_k = \left[ \frac{\gamma^{\text{RRE}}_{k-1}}{0} \right],$$  \hspace{1cm} (3.15)

which, together with (2.6), gives (3.10).

**Proof of part 2:** By (3.10) and (2.8), we have

$$s^{\text{RRE}}_k = x_0 + U_{k-1}\xi^{\text{RRE}}_k = x_0 + U_{k-2}\xi^{\text{RRE}}_{k-1} = s^{\text{RRE}}_{k-1},$$ \hspace{1cm} (3.16)

from which

$$U_{k-1}\xi^{\text{RRE}}_k = U_{k-2}\xi^{\text{RRE}}_{k-1} \Rightarrow U_{k-1}\xi^{\text{RRE}}_k = U_{k-1} \left[ \frac{\xi^{\text{RRE}}_{k-1}}{0} \right].$$ \hspace{1cm} (3.17)

By the fact that $U_{k-1}$ is of full column rank, (3.17) implies that

$$\xi^{\text{RRE}}_k = \left[ \frac{\xi^{\text{RRE}}_{k-1}}{0} \right],$$ \hspace{1cm} (3.18)

which, when combined with the relation $[\xi_j] = \sum_{i=j+1}^{k} \gamma_i$, by which, $\xi_{k-1} = \gamma_k$ in (2.7), gives (3.15). Multiplying both sides of (3.15) on the left by $R_k$, we obtain

$$R_k \gamma^{\text{RRE}}_k = \left[ \frac{R_{k-1}\gamma^{\text{RRE}}_{k-1}}{0} \right] \Rightarrow \|R_k \gamma^{\text{RRE}}_k\| = \|R_{k-1}\gamma^{\text{RRE}}_{k-1}\|. \hspace{1cm} (3.19)$$

Substituting (3.19) in (3.8), we obtain $\hat{e}_k^T c = 0$, and this completes the proof. \[\blacksquare\]

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

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

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

$$\frac{1}{[U_k \gamma^{\text{RRE}}_k]^2} = \frac{1}{[U_{k-1} \gamma^{\text{RRE}}_{k-1}]^2} + \frac{1}{[U_k \gamma^{\text{MPE}}_k]^2}, \hspace{1cm} (3.20)$$

and

$$\frac{U_k \gamma^{\text{RRE}}_k}{[U_k \gamma^{\text{RRE}}_k]^2} = \frac{U_{k-1} \gamma^{\text{RRE}}_{k-1}}{[U_{k-1} \gamma^{\text{RRE}}_{k-1}]^2} + \frac{U_k \gamma^{\text{MPE}}_k}{[U_k \gamma^{\text{MPE}}_k]^2}. \hspace{1cm} (3.21)$$

Consequently, we also have

$$\frac{s^{\text{RRE}}_k}{[U_k \gamma^{\text{RRE}}_k]^2} = \frac{s^{\text{RRE}}_{k-1}}{[U_{k-1} \gamma^{\text{RRE}}_{k-1}]^2} + \frac{s^{\text{MPE}}_k}{[U_k \gamma^{\text{MPE}}_k]^2}. \hspace{1cm} (3.22)$$

In addition,

$$[U_k \gamma^{\text{RRE}}_k] < [U_{k-1} \gamma^{\text{RRE}}_{k-1}]. \hspace{1cm} (3.23)$$
Proof. Since $s_k^{\text{MPE}}$ exists, we have $e_k^T c \neq 0$. Taking the norm of both sides in (3.8), and observing that the two terms on the right-hand side are orthogonal to each other, we first obtain

$$
\frac{1}{\|R_k\gamma_k^{\text{RRE}}\|^2} = \frac{1}{\|R_{k-1}\gamma_{k-1}^{\text{RRE}}\|^2} + \left(\frac{|e_k^T c|}{r_{kk}}\right)^2,
$$

(3.24)

which, upon invoking (3.3), gives

$$
\frac{1}{\|R_k\gamma_k^{\text{RRE}}\|^2} = \frac{1}{\|R_{k-1}\gamma_{k-1}^{\text{RRE}}\|^2} + \frac{1}{\|R_k\gamma_k^{\text{MPE}}\|^2}.
$$

(3.25)

The result in (3.20) follows from (3.25) and (3.1).

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

$$
\frac{1}{\|R_k\gamma_k^{\text{RRE}}\|^2}R_k\gamma_k^{\text{RRE}} = \frac{1}{\|R_{k-1}\gamma_{k-1}^{\text{RRE}}\|^2} \begin{bmatrix} R_{k-1}\gamma_{k-1}^{\text{RRE}} \\ 0 \end{bmatrix} + \frac{1}{\|R_k\gamma_k^{\text{MPE}}\|^2}R_k\gamma_k^{\text{MPE}}.
$$

(3.26)

Multiplying both sides of (3.26) on the left by $Q_k$, and invoking (3.1) and

$$
Q_k \begin{bmatrix} R_{k-1}\gamma_{k-1}^{\text{RRE}} \\ 0 \end{bmatrix} = \begin{bmatrix} R_{k-1}\gamma_{k-1}^{\text{RRE}} \\ 0 \end{bmatrix} = Q_{k-1}(R_{k-1}\gamma_{k-1}^{\text{RRE}}) = U_{k-1}\gamma_{k-1}^{\text{RRE}},
$$

(3.27)

we obtain (3.21).

Let us rewrite (3.21) in the form

$$
\frac{1}{\|U_k\gamma_k^{\text{RRE}}\|^2}U_k\gamma_k^{\text{RRE}} = \frac{1}{\|U_{k-1}\gamma_{k-1}^{\text{RRE}}\|^2}U_k \begin{bmatrix} \gamma_{k-1}^{\text{RRE}} \\ 0 \end{bmatrix} + \frac{1}{\|U_k\gamma_k^{\text{MPE}}\|^2}U_k\gamma_k^{\text{MPE}}.
$$

(3.28)

From (3.28) and by the fact that $U_k$ is of full column rank, it follows that

$$
\frac{1}{\|U_k\gamma_k^{\text{RRE}}\|^2}\gamma_k^{\text{RRE}} = \frac{1}{\|U_{k-1}\gamma_{k-1}^{\text{RRE}}\|^2} \begin{bmatrix} \gamma_{k-1}^{\text{RRE}} \\ 0 \end{bmatrix} + \frac{1}{\|U_k\gamma_k^{\text{MPE}}\|^2}\gamma_k^{\text{MPE}},
$$

(3.29)

and this, together with (2.6), gives (3.22).

Finally, (3.28) follows directly from (3.20). \hfill \Box

The following facts can be deduced directly from (3.20):

$$
\|U_k\gamma_k^{\text{MPE}}\| = \frac{\|U_k\gamma_k^{\text{RRE}}\|}{\sqrt{1 - \|U_k\gamma_k^{\text{RRE}}\|^2/\|U_{k-1}\gamma_{k-1}^{\text{RRE}}\|^2}} \quad \text{when } s_k^{\text{MPE}} \text{ exists.}
$$

(3.30)

$$
\frac{1}{\|U_k\gamma_k^{\text{RRE}}\|^2} = \sum_{i \in S_k} \frac{1}{\|U_i\gamma_i^{\text{MPE}}\|^2}; \quad S_k = \{0 \leq i \leq k : s_i^{\text{MPE}} \text{ exists}\}.
$$

(3.31)

Let us go back to the case in which $\{x_m\}$ is generated as in $x_{m+1} = f(x_m)$, $m = 0, 1, \ldots$, from the system $x = f(x)$. As we have already noted, with the residual associated with an arbitrary vector $x$ defined as $r(x) = f(x) - x$, (i) $U_k\gamma_k = r(s_k)$ when $f(x)$ is linear, and (ii) $U_k\gamma_k \approx r(s_k)$ when $f(x)$ is nonlinear and $s_k$ is close to
the solution $s$ of $x = f(x)$. Then, Theorem 3.2 [especially (3.30)] 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 $\phi^\text{MPE}_k = [U_k \gamma^\text{MPE}_k]$ and $\phi^\text{RRE}_k = [U_k \gamma^\text{RRE}_k]$, and recalling that $\phi^\text{RRE}_k / \phi^\text{RRE}_{k-1} \leq 1$ for all $k$, we have the following: (i) When $\phi^\text{RRE}_k / \phi^\text{RRE}_{k-1}$ is significantly smaller than 1, which means that RRE is performing well, $\phi^\text{MPE}_k$ is close to $\phi^\text{RRE}_k$, that is, MPE is performing well too, and (ii) when $\phi^\text{MPE}_k$ is increasing, that is, MPE is performing poorly, $\phi^\text{RRE}_k / \phi^\text{RRE}_{k-1}$ is approaching 1, that is, RRE is performing poorly too. Thus, when the graph of $\phi^\text{MPE}_k$ has a peak for $k_1 \leq k \leq k_2$, then the graph of $\phi^\text{RRE}_k$ has a plateau for $k_1 \leq k \leq k_2$. 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 $x = Tx + d$, where the matrix $(I - T)$ is nonsingular, and generate $\{x_m\}$ via $x_{m+1} = Tx_m + d$, $m = 0, 1, \ldots$, with some initial vector $x_0$. Apply MPE and RRE to $\{x_m\}$ to obtain the vectors $s_k$ as before. As already stated, $U_k \gamma_k = r_k = r(s_k)$, where $r(x) = (Tx + d) - x$ is the residual vector for the system $(I - T)x = d$ associated with $x$. In this case, we have the next theorem as a corollary of Theorems 3.1 and 3.2.

**Theorem 4.1** Let the sequence $\{x_m\}$ be generated recursively via $x_{m+1} = Tx_m + d$, $m = 0, 1, \ldots$, the matrix $(I - T)$ being nonsingular. Let also $r(x) = Tx + d - x$ be the residual vector corresponding to $x$. Let $k_0$ be the degree of the minimal polynomial of $T$ with respect to $u_0 = x_1 - x_0$. Then, for $k < k_0$, the vectors $s^\text{MPE}_k$ and $s^\text{RRE}_k$ obtained by applying MPE and RRE to $\{x_m\}$ and their residual vectors $r(s^\text{MPE}_k) = r^\text{MPE}_k$ and $r(s^\text{RRE}_k) = r^\text{RRE}_k$ satisfy the following for this special case:

1. $s^\text{RRE}_k = s^\text{RRE}_{k-1}$ if and only if $s^\text{MPE}_k$ fails to exist.

2. In case $s^\text{MPE}_k$ exists, there hold

$$\frac{1}{\|r^\text{RRE}_k\|^2} = \frac{1}{\|r^\text{RRE}_{k-1}\|^2} + \frac{1}{\|r^\text{MPE}_k\|^2}. \quad (4.1)$$

$$\frac{s^\text{RRE}_k}{\|r^\text{RRE}_k\|^2} = \frac{s^\text{RRE}_{k-1}}{\|r^\text{RRE}_{k-1}\|^2} + \frac{s^\text{MPE}_k}{\|r^\text{MPE}_k\|^2}. \quad (4.2)$$

Consequently, we also have

$$\frac{s^\text{RRE}_k}{\|r^\text{RRE}_k\|^2} = \frac{s^\text{RRE}_{k-1}}{\|r^\text{RRE}_{k-1}\|^2} + \frac{s^\text{MPE}_k}{\|r^\text{MPE}_k\|^2}. \quad (4.3)$$

In addition,

$$[r^\text{RRE}_k] < [r^\text{RRE}_{k-1}]. \quad (4.4)$$
3. \( s_{k_0}^{MPE} = s_{k_0}^{RRE} = s \), where \( s \) is the solution to \((I - T)x = d\).

In view of (4.1), the results in (3.30) and (3.31) become

\[
\begin{bmatrix} r_k^{MPE} \end{bmatrix} = \frac{\begin{bmatrix} r_k^{RRE} \end{bmatrix}}{\sqrt{1 - (\|r_k^{RRE}\|/\|r_{k-1}^{RRE}\|)^2}} \quad \text{when } s_k^{MPE} \text{ exists} \tag{4.5}
\]

and

\[
\frac{1}{\|r_k^{RRE}\|^2} = \sum_{i \in S_k} \frac{1}{\|r_i^{MPE}\|^2} ; \quad S_k = \{0 \leq i \leq k : s_i^{MPE} \text{ exists}\} \tag{4.6}
\]

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

Theorem 2.4 in [21] concerns the mathematical equivalence of vector extrapolation methods to Krylov subspace methods, when all these methods are defined using the standard 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 \(\{x_m\} \) obtained via \(x_{m+1} = Tx_m + d\), \(m = 0, 1, \ldots\), with some \(x_0\), and
- FOM and GMR are being applied to \((I - T)x = d\), starting with the same initial vector \(x_0\).

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 \((\cdot, \cdot)\) and the weighted norm \(\|\cdot\|\) induced by \((\cdot, \cdot)\).

For the solution of a nonsingular linear system \(Ax = b\), whose solution we denote by \(s\), FOM and GMR construct their approximations \(w_k\) as follows: Define the residual vector corresponding to \(x\) by \(r(x) = b - Ax\) and denote \(r_0 = r(x_0)\) for some initial vector \(x_0\). Let \(K_k(A; r_0) = \text{span}\{r_0, Ar_0, \ldots, A^{k-1}r_0\}\). Then, for each method, the approximation \(w_k\) to \(s\) is of the form \(w_k = x_0 + y\) such that \(y \in K_k(A; r_0)\), and \(y\) is the vector to be determined. Using the weighted inner product \((\cdot, \cdot)\) and the norm \(\|\cdot\|\) induced by \((\cdot, \cdot)\), these methods can be redefined as follows:

- For FOM, \(y\) is determined by requiring that \((z, r_k^{FOM}) = 0\) for all \(z \in K_k(A; r_0)\), where \(r_k^{FOM} = r(w_k^{FOM})\).

- For GMR, \(y\) is determined by requiring that \(\|r_k^{GMR}\| = \min_{y \in K_k(A; r_0)} \|r(x_0 + y)\|\), where \(r_k^{GMR} = r(w_k^{GMR})\).

Then we have the following generalization of Theorem 2.4 in [21]:
Theorem 4.2 Consider the nonsingular linear system \((I - T)x = d\). Apply FOM and GMR to this system starting with some initial vector \(x_0\). Apply MPE and RRE to the sequence \(\{x_m\}\) obtained from \(x_{m+1} = Tx_m + d\), \(m = 0, 1, \ldots\), with the same initial vector \(x_0\). Then

\[
\mathbf{w}_k^{\text{FOM}} = s_k^{\text{MPE}} \quad \text{and} \quad \mathbf{w}_k^{\text{GMR}} = s_k^{\text{RRE}},
\]

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 \(\mathbf{w}_k^{\text{FOM}}\) and \(\mathbf{w}_k^{\text{GMR}}\).

**Proof.** The same as that of [21, Theorem 2.4]. \(\blacksquare\)

These results for FOM and GMR are not new. They were given originally by Weiss [31] and by Brown [4], and developed further in the papers mentioned in Section [1].

Note that the vectors \(\mathbf{w}_k^{\text{FOM}}\) and \(\mathbf{w}_k^{\text{GMR}}\) can be obtained numerically by modifying the known algorithms for FOM and GMR via the introduction of the weighted QR factorization in the Arnoldi–Gram–Schmidt process, in exactly the same way we have approached the problem of computing \(s_k^{\text{MPE}}\) and \(s_k^{\text{RRE}}\), the rest being simple.

**Appendix: Weighted QR factorization**

**A.1 Gram–Schmidt process and existence and uniqueness of the weighted QR factorization**

*Gram-Schmidt orthogonalization*, also called the *Gram-Schmidt process* (GS), is a procedure that takes an arbitrary set of linearly independent vectors \(\{a_1, \ldots, a_s\}\) and constructs a set of vectors \(\{q_1, \ldots, q_s\}\) out of them, such that the \(q_i\) are orthonormal with respect to some specified inner product. In addition, the \(q_i\) are generated in a way that ensures

\[
\text{span}\{a_1, \ldots, a_j\} = \text{span}\{q_1, \ldots, q_j\}, \quad j = 1, \ldots, s.
\]

This, of course, implies

\[
a_1 = r_{11}q_1
\]
\[
a_2 = r_{12}q_1 + r_{22}q_2
\]
\[
a_3 = r_{13}q_1 + r_{23}q_2 + r_{33}q_3
\]

\[\vdots\]
\[
a_s = r_{1s}q_1 + r_{2s}q_2 + \cdots + r_{ss}q_s,
\]

for some suitable scalars \(r_{ij}\).

**Remark:** We observe that, with \(a_i, q_i \in \mathbb{C}^m\), the relationships in (A.1), with no conditions imposed on the \(q_j\) and \(r_{ij}\), can be expressed in matrix form as in

\[
A = QR,
\]

(A.2)
where
\[ A = [a_1 | a_2 | \cdots | a_s] \in \mathbb{C}^{m \times s} \tag{A.3} \]
and
\[ Q = [q_1 | q_2 | \cdots | q_s] \in \mathbb{C}^{m \times s}, \quad R = \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1s} \\ r_{21} & r_{22} & \cdots & r_{2s} \\ \vdots & \vdots & \ddots & \vdots \\ r_{s1} & r_{s2} & \cdots & r_{ss} \end{bmatrix} \in \mathbb{C}^{s \times s}. \tag{A.4} \]

By this, we mean that (A.2)–(A.4) follow directly from (A.1), in which the vectors \( q_j \) and the scalars \( r_{ij} \) are not required to satisfy any specific conditions except (A.1) itself.

Let \( \langle \cdot, \cdot \rangle \) be a weighted inner product in \( \mathbb{C}^m \), given as
\[ \langle y, z \rangle = y^* G z, \quad G \in \mathbb{C}^{m \times m} \text{ hermitian positive definite}, \]
and let \( \| \cdot \| \) be the norm induced by \( \langle \cdot, \cdot \rangle \), given as
\[ \| z \| = \sqrt{\langle z, z \rangle} = \sqrt{z^* G z}. \]

We now return to the determination via GS of the \( q_j \) and the \( r_{ij} \) such that the \( q_i \)s satisfy the orthogonality condition \( \langle q_i, q_j \rangle = \delta_{ij} \). The first of the relations in (A.1) gives \( r_{11} \) and \( q_1 \) as follows:
\[ r_{11} = \| a_1 \|, \quad q_1 = a_1 / r_{11}. \]

With \( q_1 \) determined, and by invoking the requirement that \( \langle q_1, q_2 \rangle = 0 \), the second relation is used to determine \( r_{12}, r_{22} \), and \( q_2 \) as in
\[ r_{12} = \langle q_1, a_2 \rangle, \quad \tilde{a}_2 = a_2 - r_{12} q_1, \quad r_{22} = \| \tilde{a}_2 \|, \quad q_2 = \tilde{a}_2 / r_{22}. \]

We now proceed in the same way and determine \( q_3, \ldots, q_s \) and the rest of the \( r_{ij} \). For example, with \( q_1, \ldots, q_{j-1} \) already determined and \( \langle q_i, q_j \rangle = \delta_{ij} \) for \( 1 \leq i, i' \leq j - 1 \), and by invoking the requirement that \( \langle q_i, q_j \rangle = 0 \) for \( i < j \), from the relation \( a_j = \sum_{i=1}^{j-1} r_{ij} q_i \) in (A.1), we determine \( r_{ij} \) for \( i < j \) and \( q_j \) as follows:
\[ r_{ij} = \langle q_i, a_j \rangle, \quad 1 \leq i < j; \quad \tilde{a}_j = a_j - \sum_{i=1}^{j-1} r_{ij} q_i, \quad r_{jj} = \| \tilde{a}_j \|, \quad q_j = \tilde{a}_j / r_{jj}. \]

Note that, since the \( a_i \) are linearly independent, the vectors \( \tilde{a}_j \) are nonzero and hence \( r_{jj} > 0 \) for all \( j \). Note also that \( r_{ij} q_i \) is the projection of \( a_j \) along \( q_i, i \leq j \).

Since the columns of the matrix \( Q \) are orthogonal with respect to a general inner product in \( \mathbb{C}^m \), and since the most general inner products are necessarily weighted inner products, we will call the QR factorization of \( A \) given in (A.2)–(A.4) a \textit{weighted QR factorization}. The next theorem summarizes the existence and uniqueness of the weighted QR factorization.
Theorem A.1 Let
\[ A = [a_1 | a_2 | \cdots | a_s] \in \mathbb{C}^{m \times s}, \quad m \geq s, \quad \text{rank}(A) = s. \]

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

Specifically,
\[ Q = [q_1 | q_2 | \cdots | q_s], \quad R = \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1s} \\ r_{22} & \ddots & \ddots & \ddots \\ \vdots & \ddots & \ddots & \ddots \\ r_{ss} & & & \end{bmatrix}, \]
\[ \langle q_i, q_j \rangle = q_i^* G q_j = \delta_{ij} \quad \forall \ i, j, \]
\[ r_{ij} = \langle q_i, a_j \rangle = q_i^* G a_j \quad \forall \ i \leq j; \quad r_{ii} > 0 \quad \forall \ i. \]

In addition, the matrices \( Q \) and \( R \) are unique.

Proof. Clearly, the columns of \( Q \) and the entries of \( R \) are precisely those in (A.1), as provided by the Gram–Schmidt orthogonalization we have just described, with the inner product \( \langle \cdot, \cdot \rangle \). We have thus shown the existence of the QR factorization for \( A \). [Recall also the remark following (A.1).]

We now turn to the proof of uniqueness. Suppose that \( A = Q_1 R_1 \) and \( A = Q_2 R_2 \) are two QR factorizations. Then, by \( Q_1 R_1 = Q_2 R_2 \), we have both \( R_1 R_2^{-1} = Q_1^* G Q_2 \) and \( R_2 R_1^{-1} = Q_2^* G Q_1 \). Since \( R_1 R_2^{-1} \) and \( R_2 R_1^{-1} \) are both upper triangular with positive diagonals, so are \( Q_1^* G Q_2 \) and \( Q_2^* G Q_1 \). But \( Q_1^* G Q_2 = (Q_2^* G Q_1)^* \), and hence \( Q_1^* G Q_2 \) is lower triangular as well; therefore, \( Q_1^* G Q_2 \) is diagonal with positive diagonal elements. So is \( Q_2^* G Q_1 \). Now, \( Q_1^* G Q_2 \) is unitary since
\[ (Q_1^* G Q_2)^* (Q_1^* G Q_2) = (Q_2^* G Q_1) (Q_1^* G Q_2) = (R_2 R_1^{-1}) (R_1 R_2^{-1}) = I_s. \]

Since the only diagonal unitary matrix with positive diagonal elements is \( I_s \), we have \( Q_1^* G Q_2 = I_s \). Similarly, we have \( Q_2^* G Q_1 = I_s \). Therefore,
\[ R_1 R_2^{-1} = I_s = R_2 R_1^{-1}, \quad \text{hence} \quad R_1 = R_2. \]

As a result,
\[ Q_1 = A R_1^{-1} = A R_2^{-1} = Q_2. \]

This completes the proof.

Remark. The weighted QR factorization of Theorem A.1 reduces to the standard QR factorization when \( G = I_m \), that is, when \( \langle \cdot, \cdot \rangle \) is the standard Euclidean inner product \( \langle y, z \rangle = y^* z \). In this case, \( Q \) is a unitary matrix in the regular sense, that is, \( Q^* Q = I_s \).
A.2 Weighted QR factorization by the modified Gram–Schmidt process

It is well known that, in floating-point arithmetic, the orthogonalization process [with the standard inner product \( \langle y, z \rangle = y^\ast z \)] via GS is very inaccurate, and that this problem can be fixed to a large extent by using the modified Gram–Schmidt process (MGS) in order to overcome numerical instabilities. In view of this, it seems reasonable to suggest that MGS would be preferable to GS with the weighted inner product \( \langle y, z \rangle = y^\ast Gz \) too, even though the (numerical) end result may be influenced by the matrix \( G \). Here are the steps of MGS:

MGS Algorithm

MGS1. Set \( r_{11} = \|a_1\| \) and \( q_1 = a_1/r_{11}. \)

MGS2. For \( j = 2, \ldots, s \) do

Set \( a_j^{(1)} = a_j. \)

For \( i = 1, \ldots, j - 1 \) do

Compute \( r_{ij} = \langle q_i, a_j^{(i)} \rangle \) and compute \( a_j^{(i+1)} = a_j^{(i)} - r_{ij}q_i. \)

end do \((i)\)

Compute \( r_{jj} = \|a_j^{(j)}\| \) and set \( q_j = a_j^{(j)}/r_{jj}. \)

end do \((j)\)

It is easy to show that, in exact arithmetic, the scalars \( r_{ij} \) and the vectors \( q_j \) computed by MGS are the same as those computed by GS. Comparing the GS and MGS algorithms, we also see that their costs are identical. However, they differ in the way they compute the \( r_{ij} \) [namely, \( r_{ij} = \langle q_i, a_j \rangle \) for GS, while \( r_{ij} = \langle q_i, a_j^{(i)} \rangle \) for MGS, the rest of the computations being identical], and this may have a hopefully beneficial effect on the rest of the computation. For example, once \( r_{13}q_1 \), the projection of \( a_3 \) along \( q_1 \), has been computed, it is immediately subtracted from \( a_3^{(1)} = a_3 \) to give \( a_3^{(2)} \) and then \( r_{23} \) is computed via \( \langle q_2, a_3^{(2)} \rangle \) instead of \( \langle q_2, a_3 \rangle \), even though they are equal mathematically speaking.

Before closing, we mention that weighted QR factorizations are discussed in great detail by Gulliksson and Wedin [12] and Gulliksson [11]. These papers discuss the use of MGS and also of suitable generalizations of Householder reflections in computing the weighted QR factorization. Numerical aspects of this computation for diagonal matrices \( G = \text{diag}(\alpha_1, \ldots, \alpha_s), \alpha_i > 0 \ \forall \ i, \) are studied in [11] for different relative sizes of the \( \alpha_i. \)

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