Abstract. Rational Krylov subspace projection methods are one of successful methods in MOR, mainly because some order derivatives of the approximate and original transfer functions are the same. This is the well known moments matching result. However, the properties of points which are far from the interpolating points are little known. In this paper, we obtain the error’s explicit expression which involves shifts and Ritz values. The advantage of our result over than the known moments matches theory is, to some extent, similar to the one of Lagrange type remainder formula over than Peano Type remainder formula in Taylor theorem. Expect for the proof, we also provide three explanations for the error formula. One explanation shows that in the Gauss-Christoffel quadrature sense, the error is the Gauss quadrature remainder, when the Gauss quadrature formula is applied onto the resolvent function. By using the error formula, we propose some greedy algorithms for the interpolatory $H_\infty$ norm MOR.

Key words. transfer function, rational Krylov subspace, Ritz value, $H_\infty$ model order reduction

AMS subject classifications. 34C20, 41A05, 49K15, 49M05, 93A15, 93C05, 93C15

1. Introduction. We are interested in the model error of model order reduction (MOR) [61] by rational Krylov subspace projection methods. The origin single-input-single-output (SISO) dynamical system is:

$$\begin{cases}
\frac{dx(t)}{dt} = Ax(t) + bu(t), \\
y(t) = c^H x(t),
\end{cases}$$

with $A \in \mathbb{C}^{n \times n}$ and $b, c \in \mathbb{C}^{n \times 1}$.

With the rational Krylov subspaces $\text{span}(V)$ and $\text{span}(W)$, we obtain the reduced system:

$$\begin{cases}
WHV \frac{dx(t)}{dt} = WHAVx(t) + WHbu(t), \\
y(t) = c^H Vx(t).
\end{cases}$$

Their transfer functions are

$$h(z) = c^H (zI - A)^{-1}b,$$
$$\tilde{h}(z) = c^H V(zWHV - WHAV)^{-1}WHb.$$
In 1997, Grimme [33] already noticed the model error can be expressed by $e(z) = r_c^H(zI - A)^{-1}r_b$. This truth is used in later references (e.g. [5, 6, 22, 23, 55]). Our work begins by expanding $r_b$ and $r_c$ with respect to the Ritz values and the shifts. The expressions of the residual $r$ by rational Krylov subspace methods are provided by [9, 19, 36, 41, 64]. The known expressions of the residual are Galerkin type (one-sided) projection. When we generalize it for dealing with MOR, we replace it by Petro-Galerkin (two-sided) projection, which is a common manner of MOR. Thus, we obtain an expression of $e(z)$.

Note the Ritz values are the quadrature nodes of Gauss-Christoffel quadrature. This motivates our working on finding the relation between the error formula and the Gauss quadrature. The book [46, Chapter 3] by Liesen and Strakoš reveals the relating theory for Hermitian $A$ and $b = c$. After some derivations, we observe that the error formula is actually the Gauss quadrature remainder, when the Gauss quadrature formula is applied onto the resolvent function $H(\lambda, z) = 1/(z - \lambda)$.

With the information of the previous proofs, we also notice the error formula is actually the interpolation remainder, when Hermitian formula is applied onto the resolvent function with respect to variables $z$ and $\lambda$. Thus, we obtain the second and third explanations. Because of these explanations, we also call $e(z)$ as the transfer function interpolation remainder.

It deserves further researching that how it relates to the other parts of MOR. One of the most interesting problems is the interpolatory $H_\infty$ norm MOR. By using the remainder formula, we can transform the $H_\infty$ norm MOR into the approximation of the operator functions. The later work is already well established by Güttel [35–37]. His approach is based on an estimation of Walsh-Hermite formula. When our problem involves the resolvent function $H(\lambda, z)$, it is quite special, since the Cauchy integral in Walsh-Hermite formula is computed successfully. After looking more closely at the error formula, we get some approximations which can be computed in reduced problems. Then, our greedy algorithms are designed and compared with other MOR algorithms. Numerical experiment shows its error in $H_\infty$ norm has the similar behavior as the one of IRKA (which computes $H_2$ norm MOR), but our algorithms need much less CPU times.

The paper is structured as follows: In Section 2, we present our expression of the error $e(z)$ with one proof and another three explanations. After noticing the remainder of the $l$ order two-sided projection MOR has the similar form as the $2l$ order one-sided projection MOR, we also provide the remainder formula of $2l$ order one-sided projection MOR in Section 3. In Section 4, we discuss the interpolatory $H_\infty$ norm MOR and give some approximations of $e(z)$. In section 5, we propose some greedy algorithms by modifying [19]. In Section 6, we do numerical testing for benchmark problems. We list our main contributions in Section 7.

**Notation:** The standard Krylov subspace is denoted by

$$\text{Krylov}(A, b, l) := \text{span}(b, Ab, \ldots, A^{l-1}b).$$

(1.1)

The shifts sets for the left and right rational Krylov subspaces are respectively denoted by $T = \{t_j\}_{j=1}^{k_t}$ and $S = \{s_j\}_{j=1}^{k_s}$. Hence, the rational Krylov subspaces are written by

$$\text{RK}(A, b, S, k_b) := \text{span}\{(A - s_1I)^{-1}b, (A - s_2I)^{-1}b, \ldots, (A - s_{k_s}I)^{-1}b\},$$

$$\text{RK}(A^H, c, T, k_c) := \text{span}\{(A - t_1I)^{-H}c, (A - t_2I)^{-H}c, \ldots, (A - t_{k_t}I)^{-H}c\}.$$  

(1.2)

$\mathbb{P}_m(\lambda)$ denotes the polynomial set, in which the degree of the polynomials is less than or equal to $m$. Given $\varphi(\lambda)$, the symbol $\mathbb{P}_m(\lambda)/\varphi(\lambda)$ denotes the rational polynomial set. The numerator of its element is a polynomial, whose degree is less than or equal to $m$. The symbol $\mathbb{Q}_{l-1, l}(\lambda)$ also denotes the rational polynomial set. The numerator of its element is of $l - 1$ degree, while the denominator is of $l$ degree.

Write $t = \sqrt{-1}$. Let $\text{eig}(A) = \{\lambda_i(A)\}_{i=1}^n$ denotes the set of $A$’s eigenvalues. The field of values of $A$ is defined as $\mathcal{W}(A) = \{x^HAx : x \in \mathbb{C}^n, x^Hx = 1\}$. The uniform norm of a function on a set $\Sigma$ is defined by
The operation \( \text{orth}(V) \) gets the orthonormal basis matrix of \( \text{span}(V) \). Unless otherwise specified, the norm \( \| \cdot \| \) is an abbreviation of \( \| \cdot \|_2 \). Whenever possible, Matlab notation will be used.

2. The error formula by two-sided projection. We first define the combined Krylov (CK) subspaces.

\[
\begin{align*}
\text{CK}(A, b, k_b, m_b) & := \text{RK}(A, b, S, k_b) \cup \text{Krylov}(A, b, m_b), \\
\text{CK}(A^H, c, k_c, m_c) & := \text{RK}(A^H, c, \mathbf{T}, k_c) \cup \text{Krylov}(A^H, c, m_c),
\end{align*}
\]

(2.1)

where (rational) Krylov subspaces are defined by (1.1) and (1.2). With notations \( l := k_b + m_b = k_c + m_c \) and

\[
\varphi(z) := \prod_{j=1}^{k_b} (z - s_j), \quad \psi(z) := \prod_{j=1}^{k_c} (z - t_j),
\]

(2.2)

we observe that (cf. Section 2.2.1)

\[
\text{CK}(A, b, k_b, m_b) = \text{Krylov}(A, \varphi(A)^{-1}b, l), \quad \text{CK}(A^H, c, k_c, m_c) = \text{Krylov}(A^H, \psi(A)^{-1}c, l).
\]

Theorem 2.1. Let \( V \) and \( W \) satisfy \( \text{span}(V) = \text{CK}(A, b, k_b, m_b), \text{span}(W) = \text{CK}(A^H, c, k_c, m_c) \) defined by (2.1). Suppose that Lanczos biorthogonalization procedure of \([A, \varphi(A)^{-1}b, \psi(A)^{-1}c] \) does not break until \((l+1)\)th iteration. Let \( \Lambda(\lambda) := \prod_{i=1}^{l} (\lambda - \lambda_i) \) be the monic characteristic polynomial of \((W^H V)^{-1} W^H A V\). With (2.2), write

\[
g_b(\lambda) := \frac{\Lambda(\lambda)}{\varphi(\lambda)}, \quad g_c(\lambda) := \frac{\Lambda(\lambda)}{\psi(\lambda)}.
\]

(2.3)

Then, it holds that

\[
e(z) = h(z) - \tilde{h}(z) = e^H(zI - A)^{-1}b - e^H V(z W^H V - W^H A V)^{-1} W^H b
\]

\[
= \frac{1}{g_b(z) g_c(z)} e^H g_c(A)(zI - A)^{-1} g_b(A) b.
\]

The proof is divided into three steps: Theorem 2.5, Theorem 2.12 and the final proof in Section 2.3. Furthermore, we have Theorem 2.19 for the generalization onto the descriptor system. The proof is a constructive type one by using a Lanczos biorthogonalization procedure. The involving assumption ensures \( W^H V \) is nonsingular.

Now, we give some remarks immediately.

1. The combined Krylov subspaces span the same subspaces as [27, Definition 11]. Our bases in the definition (2.1) are product type bases, with no consideration on the multiplicity of the shifts. This type basis is a truncation of the one used in [44, Theorem 6.1]. These bases are one of various bases of rational Krylov subspace. By the expressions of (rational) polynomials (e.g. [36, Lemma 4.2(d)]), they are easily known to span the same subspace.

2. Note that \( k_b + m_b = k_c + m_c \), but \( k_b \) does not need to be equal to \( k_c \). We set up our rational subspace as common as possible, so that we can include the majority of the interesting subspaces. The theorem is a conclusive result of the interpolation property. It directly gives rise to the moments matching results (e.g. [1, Proposition 11.7, Proposition 11.8, Proposition 11.10, Proposition 11.11]). From the form of \( e(z) \) in Theorem 2.1, it is easy to check that \( e(z) \) perfectly satisfies [27, Definition 16] (an equivalent condition of moments matching).

3. It is observed that the Krylov subspace type methods can not maintain the stability of the system. By Theorem 2.1, we easily get the reason. The error formula is independent of the stability of \( A \). Specifically, the condition of Theorem 2.1 does not require \( \text{eig}(A) \) be in the left half plane. Thus, we can not expect this two-sided projection method to maintain the stability, unless we add more constrains. Note that there exist some other applications which do not involve the stability of \( A \) (e.g. [14, (3.4)] [49, Theorem 3.1]).
2.1. Step 1: Special subspaces and special bases. We first prove a special case of Theorem 2.1 when \( l = m_b = m_c =: m, k_b = k_c = 0 \). The main result of this step is Theorem 2.5.

2.1.1. Lanczos biorthogonalization procedure. Our proof uses the bases from the Lanczos biorthogonalization procedure of \((A, b, c)\) [e.g., [60, Section 7.1]]. Thus, we need the assumption that the procedure does not break out. The conditions of successfully executing procedure are well researched (a recent work [56]). The relations from the Lanczos biorthogonalization procedure of \((A, b, c)\) are concluded by:

\[
v_1 = b, \quad w_1 = c, \quad c^H b = 1, \\
A V_m = V_{m+1} T_n, \quad \text{span}(V_m) = \text{Krylov}(A, b, m), \quad \text{span}(V_{m+1}) = \text{Krylov}(A, b, m + 1), \\
A^H W_m = W_{m+1} \mathcal{K}_n, \quad \text{span}(W_m) = \text{Krylov}(A^H, c, m), \quad \text{span}(W_{m+1}) = \text{Krylov}(A^H, c, m + 1), \\
W_m^H V_m = I, \quad W_{m+1}^H V_{m+1} = I, \quad W_m^H A V_m = T_m, \quad V_{m+1}^H A^H W_m = K_m, \quad T_m = K_m^H,
\]

(2.4)

**Lemma 2.2.** Let \( \tau_j(\lambda) = a_j^0 \lambda^j + a_{j-1}^1 \lambda^{j-1} + \cdots + a_0^j \lambda + a_0^0 \) be a polynomial of degree \( j \). It is easy to see that \( \tau_j(A)b \in \text{Krylov}(A, b, j + 1) \) and \( \tau_j(A)b \notin \text{Krylov}(A, b, j) \). With the basis \( V \) in (2.4), we have

\[
\tau_j(A)b = V_m \tau_j(T_m)e_1, \quad j < m
\]

(2.5)

\[
\tau_m(A)b = V_m \tau_m(T_m)e_1 + a_m^m \zeta_m v_{m+1}, \quad j = m
\]

(2.6)

where \( \zeta_m = \gamma_{m+1} \cdots \gamma_2 \gamma_1 \).

**Lemma 2.3.** Suppose relations (2.4) hold. Let \( r \) be a nonzero vector, which is in \( \text{Krylov}(A, b, m + 1) \) and orthogonal to \( \text{Krylov}(A^H, c, m) \). Then \( r = \rho \lambda_m(A)b \), where \( \rho \neq 0 \) and \( \lambda_m(\lambda) = \det(\lambda I - T_m) \) is the monic characteristic polynomial of \( T_m \).

The above lemmas are generalizations of [31, Lemma 3.1, Lemma 3.2] or [54, Lemma 2.1, Corollary 2.1]. Since the proofs are quite similar, we do not provide the details.

2.1.2. The derivation. Similar to the case of the linear equation [60, Chapter 5], we require the residual be orthogonal to the given subspace. With notations

\[
r_b := b - (zI - A)x_b, \quad r_c := c - (zI - A)^H x_c,
\]

(2.7)

we have projection (Petro-Galerkin) condition:

\[
x_b \in \text{Krylov}(A, b, m) = \text{span}(V_m), \quad \text{s.t.} \quad r_b \perp \text{Krylov}(A^H, c, m) = \text{span}(W_m),
\]

and \( x_c \in \text{Krylov}(A^H, c, m) = \text{span}(W_m) \), \( \text{s.t.} \quad r_c \perp \text{Krylov}(A, b, m) = \text{span}(V_m) \).

Thus, we get \( h(z) = x_c^H b = c^H x_b \), where

\[
x_b = V(zI - W^H A)^{-1} W^H b, \quad x_c = W(zI - W^H A)^{-H} V^H c.
\]

With (2.7), we easily observe that: For any complex \( z \), it holds that

\[
r_b \in \text{Krylov}(A, b, m + 1) = \text{span}(V_{m+1}), \quad r_c \in \text{Krylov}(A^H, c, m + 1) = \text{span}(W_{m+1}).
\]
We define the polynomial expression:

\[ x_b = \chi_b(A, z)b, \quad \chi_b(\lambda, z) \in \mathbb{P}_{m-1}(\lambda), \]

\[ r_b = \gamma_b(A, z)b, \quad \gamma_b(\lambda, z) \in \mathbb{P}_m(\lambda). \]

Their relations are given by

\[
\begin{align*}
    r_b &= b - (zI - A)r_b, \\
    \gamma_b(\lambda, z) &= 1 - (z - \lambda)\chi_b(\lambda, z), \\
    \chi_b(\lambda, z) &= \frac{1 - \gamma_b(\lambda, z)}{z - \lambda}.
\end{align*}
\]  

(2.8)

We easily find \( \gamma_b(\lambda, z) \) satisfies a constraint condition:

\[ \gamma_b(z, z) = 1. \]  

(2.9)

Similar to \([34, (3.8)]\) and \([31, \text{Theorem 3.1}]\), we obtain the polynomial formulas for the residuals.

**Lemma 2.4.** Suppose relations (2.4) hold. Then, it holds

\[
\begin{align*}
    r_b &= \gamma_b(A, z)b, \\
    \gamma^H_c &= c^H\gamma_c(A, z), \\
    \gamma_b(\lambda, z) &= \gamma_c(\lambda, z) = \frac{\Lambda(\lambda)}{\Lambda(z)},
\end{align*}
\]

where \( \Lambda(\lambda) := \prod_{i=1}^{m} (\lambda - \lambda_i) \) is the monic characteristic polynomial of \( T_m = W^H AV \).

**Proof.** We observe that \( r_b \in \text{Krylov}(A, b, m + 1) \) and \( r_b \perp \text{Krylov}(A^H, c, m) \). By Lemma 2.3, we directly obtain \( r_b = \rho \Lambda(A)b \), where \( \Lambda(\lambda) \) is the monic characteristic polynomial of \( T_m = W^H AV \). Obviously, when \( z \) varies, \( \rho \) changes. So, we can consider \( \rho \) as the function of variable \( z \). Therefore, we get \( \gamma_b(\lambda, z) = \rho(z)\Lambda(\lambda) \).

By constraint condition (2.9), we directly obtain \( \rho(z) = 1/\Lambda(z) \) and then \( \gamma_b(\lambda, z) = \Lambda(\lambda)/\Lambda(z) \). Similarly, we get the result about \( r_c \). \( \square \)

**Theorem 2.5.** Suppose the Lanczos biorthogonalization procedure of \((A, b, c)\) does not break out until \((m + 1)\)th iteration. The relations of the formed matrices are given by (2.4). Then, it holds that

\[
\begin{align*}
    h(z) - \tilde{h}(z) &= c^H(zI - A)^{-1}b - c^H V(z W^H V - W^H AV)^{-1} W^H b \\
    &= c^H(zI - A)^{-1}b - c^H V(z I - W^H AV)^{-1} W^H b \\
    &= \frac{1}{[\Lambda(z)]^2} c^H (zI - A)^{-1} [\Lambda(A)]^2 b
\end{align*}
\]

where \( \Lambda(\lambda) := \prod_{i=1}^{m} (\lambda - \lambda_i) \) is the monic characteristic polynomial of \( T_m = W^H AV \).

**Proof.** Note that

\[
\begin{align*}
    r_b &= b - (zI - A)x_b, \\
    (zI - A)^{-1}b - x_b &= (zI - A)^{-1}r_b, \\
    c^H(zI - A)^{-1}b - c^H x_b &= c^H(zI - A)^{-1}r_b, \\
    \text{similarly,} \quad c^H(zI - A)^{-1} &= r_c^H(zI - A)^{-1} + x_c^H.
\end{align*}
\]

Since \( x_c \in \text{Krylov}(A^H, c, m) \) and \( r_b \perp \text{Krylov}(A^H, c, m) \), we know \( x_c^H r_b = 0 \). By Lemma 2.4, we obtain

\[
\begin{align*}
    e(z) &= h(z) - \tilde{h}(z) = c^H(zI - A)^{-1}b - c^H x_b = c^H(zI - A)^{-1}r_b = [r_c^H(zI - A)^{-1} + x_c^H] r_b \\
    &= r_c^H(zI - A)^{-1}r_b = c^H \frac{\Lambda(A)}{\Lambda(z)} (zI - A)^{-1} \frac{\Lambda(A)}{\Lambda(z)} b = \frac{1}{[\Lambda(z)]^2} c^H (zI - A)^{-1} [\Lambda(A)]^2 b.
\end{align*}
\]
Remark 2.6. The relation (2.4) requires $c^HHb = 1$, which is not the common case in practice. However, it actually does not influence the result of Theorem 2.5. The coefficient $m_0 := c^HHb$ is actually the first moment of $c^HA^hb$ [56, (2.1)]. Note that $h(z) = c^H(zI - A)^{-1}b = m_0c^H(zI - A)^{-1}(b/m_0)$. After applying Theorem 2.5 onto $(A, b/m_0, c)$ and multiplying the obtained result by $m_0$, we shall again get Theorem 2.5 without the assumption $c^HHb = 1$.

The relation $e(z) = r_c^H(zI - A)^{-1}r_b$ is known in Grimme’s PhD thesis [33, Theorem 5.1]. The traditional result shows that $e(z) = O(1/z^{2m+1})$ (e.g. [1, Section 11.2.1] [46, (3.3.26)]). Now, we explicitly reveal what exactly it is.

2.1.3. Explanation of the error from Gauss quadrature. Since Ritz values are the quadrature nodes of a Gauss-Christoffel quadrature, we are motivated to finding the relation between the error formula and the moments matching. Book [46, Chapter 3] by Liesen and Strakoš clearly reveals the involving relations among symmetric Lanczos procedure, moments matching, orthogonal polynomials, continued fractions and Gauss quadrature. It is for Hermitian $A$ and $b = c$. Recently, Strakoš and his co-workers have a series of work on generalizing it to Lanczos biorthogonalization procedure [56–59, 65].

We first define a linear functional [56]:

$$\mathcal{J}(\mathcal{F}) := c^HH(\mathcal{F})b.$$  \hfill (2.10)

If $A$ is Hermitian positive definite and $b = c$, then it can be expressed as an integral [46, Page 136].

With the bases from (2.4), we have the Gauss-Christoffel quadrature formula:

$$\mathcal{J}(\mathcal{F}) = \mathcal{J}_G(\mathcal{F}) + \mathcal{E}(\mathcal{F}),$$

i.e.,

$$c^HH(\mathcal{F})b = c^HV(\mathcal{F}(T_m))W^Hb + \mathcal{J}([A(\lambda)]^2\mathcal{F}[\lambda_1, \lambda_2, \ldots, \lambda_m, \lambda, \lambda]).$$  \hfill (2.11)

We express the Gauss-Christoffel quadrature formula by the matrix form $\mathcal{J}_G(\mathcal{F}) = c^HV(\mathcal{F}(T_m))W^Hb = m_0c^HH(\mathcal{F}(T_m))e_1$. A Gauss quadrature formula obviously has the common form $\mathcal{J}_G(\mathcal{F}) = \sum_{j=1}^m \omega_j \mathcal{F}(\lambda_j)$ (cf. Remark 2.16), where $\omega_j$ is the quadrature weight coefficient, and $\lambda_j$ is the quadrature node. Actually, it also has continued fraction form (e.g. [46, Section 3.3] [1, Example 11.5]). An easy way to assert that the matrix form is a Gauss type quadrature formula is as follows.

Proposition 2.7. [24, Theorem 2] Suppose relations (2.4) hold. Then, it holds that $c^HP(A)b = c^HP(T_m)e_1$ for any $P(\lambda) \in \mathbb{P}_{2m-1}$.

The relations (2.4) require $m_0 = c^HHb = 1$. If $m_0 \neq 1$, then the treatment is the same as in Remark 2.6.

Proposition 2.7 is the common property of Gauss type quadrature formula. Obviously, it holds that $\mathcal{J}(P) = \mathcal{J}_G(P)$ for any $P(\lambda) \in \mathbb{P}_{2m-1}$. If $P(\lambda) = \lambda^j(j = 1, 2, \ldots, 2m - 1)$, then Proposition 2.7 is the well known moments matching condition at infinity [1, (11.7)].

We express the quadrature error by the divided difference (see an integral form [46, (3.2.20)] for Hermitian $A$ and $b = c$) instead of the common Lagrange type remainder involving with the high derivatives and an unknown $\xi$ (e.g. [46, (3.2.21)] [13, Section 4.3]).

Remark 2.8. If all of $\lambda_i$ are real, then the divided difference remainder can be transformed into Lagrange type remainder.

$$\mathcal{F}[\lambda_1, \lambda_2, \ldots, \lambda_m, \lambda] = \frac{\mathcal{F}^{(2m)}(\xi)}{(2m)!}.$$  \hfill (2.12)

This is a well known result (e.g. [13, Exercise 3.3.20]). We can prove it by repeatedly utilizing Lagrange mean value theorem. However, the Lagrange mean value theorem can not been directly generalized onto complex field. Thus, we can not write (2.12) for complex $\lambda_i$ directly.

Note that in complex field, Lagrange interpolating polynomials, Newton interpolating polynomials and Hermite interpolating polynomials still hold with the divided differences remainder or Hermitian remainder (cf. Lemma 2.17).
Then, we shall proceed the research with resolvent function \( \mathcal{H}(\lambda, z) = 1/(z - \lambda) \). Substituting \( \mathcal{H}(\lambda, z) = 1/(z - \lambda) \) into \( \mathcal{F}(\lambda) \) in (2.11) and noticing \( W^Hb = V^He = e_1, W^HAV = T_m \), we obtain

\[
\begin{align*}
\mathcal{H}(zI - A)^{-1}b & = c^H(V(zI - W^HAV)^{-1}W^Hb + \mathcal{E}(\mathcal{H}), \\
\text{or } e(z) & = h(z) - \hat{h}(z) = \mathcal{E}(\mathcal{H}) = \mathcal{J}([\Lambda(z)]^2\mathcal{H}[\lambda_1, \lambda_1, \lambda_2, \ldots, \lambda_m, \lambda_m, \lambda])
\end{align*}
\]

(2.13)

Lemma 2.9. Set \( \mathcal{H}(\lambda) = 1/(z - \lambda) \). It holds that \( \mathcal{H}[\lambda_1, \lambda_2, \lambda_3, \ldots, \lambda_m] = 1/\prod_{i=1}^{m}(z - \lambda_i) \) for distinct \( \lambda_i(i = 1, 2, \ldots, m) \) with \( m \geq 2 \).

Proof. By using the recursive definition of the divided differences (e.g. [13, (3.8)]), we can prove it by the mathematical induction. \( \square \)

For \( \mathcal{H}(\lambda) = 1/(z - \lambda) \), we can easily check that

\[
\mathcal{H}[\lambda_1, \lambda_1, \lambda_2, \lambda_2, \ldots, \lambda_m, \lambda, \lambda] = \frac{1}{(z - \lambda) \prod_{i=1}^{m}(z - \lambda_i)^2}.
\]

(2.14)

Note that the term \([\Lambda(z)]^2 = [\prod_{i=1}^{m}(z - \lambda_i)]^2\) is independent of \( \lambda \). After we apply definition (2.10) onto (2.13) and (2.14), we shall obtain an expression of \( e(z) \), which is exactly the same as the result of Theorem 2.5.

In conclusion, the error formula of \( e(z) \) in Theorem 2.5 is the remainder of Gauss quadrature (2.11), when the Gauss quadrature is applied onto the resolvent function \( \mathcal{H}(\lambda, z) = 1/(z - \lambda) \).

In the above discussion, we overlap many closely related terminologies, such as Jacobi matrix, (formal) orthogonal polynomials and continued fractions. Their relations are well described in [36, Chapter 3]. For more details of the Gauss quadrature, we refer the readers to [18, 24, 30, 50, 62] and references therein.

2.2. Step 2: General subspaces and special bases.

2.2.1. Biorthogonal bases of \( \text{CK}(A, b, k_b, m_b) \) and \( \text{CK}(A^H, c, k_c, m_c) \). The rational Krylov subspace can be obtained by a special standard Krylov subspace (e.g. [36, Lemma 4.2(a)]). With (2.1), we have

\[
\begin{align*}
\text{CK}(A, b, k_b, m_b) & = \text{Krylov}(A, \varphi(A)^{-1}b, l), & \text{CK}(A, b, k_b, m_b + 1) & = \text{Krylov}(A, \varphi(A)^{-1}b, l + 1), \\
\text{CK}(A^H, c, k_c, m_c) & = \text{Krylov}(A^H, \psi(A)^{-H}c, l), & \text{CK}(A^H, c, k_c, m_c + 1) & = \text{Krylov}(A^H, \psi(A)^{-H}c, l + 1).
\end{align*}
\]

(2.15)

We use the Lanczos biorthogonalization procedure of \( A, \varphi(A)^{-1}b \) and \( \psi(A)^{-H}c \) to form the biorthogonal bases of \( \text{Krylov}(A, \varphi(A)^{-1}b, l + 1) \) and \( \text{Krylov}(A^H, \psi(A)^{-H}c, l + 1) \). The relations are summarized as follows.

\[
\begin{align*}
\hat{v}_1 & = \varphi(A)^{-1}b, & \hat{w}_1 & = \psi(A)^{-H}c, & \hat{w}_1^H\hat{v}_1 & = 1, \\
A\hat{v}_1 & = \hat{v}_{i+1}, & \text{span}(\hat{v}_1) & = \text{Krylov}(A, \varphi(A)^{-1}b, l), & \text{span}(\hat{v}_{i+1}) & = \text{Krylov}(A, \varphi(A)^{-1}b, l + 1) \\
A^H\hat{w}_1 & = \hat{w}_{i+1}, & \text{span}(\hat{w}_1) & = \text{Krylov}(A^H, \psi(A)^{-H}c, l), & \text{span}(\hat{w}_{i+1}) & = \text{Krylov}(A^H, \psi(A)^{-H}c, l + 1), \\
\hat{v}_1 & = I, & \hat{w}_1^H\hat{v}_1 & = I, & \hat{w}_1^H\hat{w}_{i+1} & = \hat{T}_i, & \hat{v}_i^H\hat{w}_{i+1} & = \hat{K}_i, & \hat{T}_i & = \hat{K}_i^H.
\end{align*}
\]

(2.16)

Like what is done in Section 2.1.2, we introduce the same notations for \( x_b, x_c, r_b, r_c \) and their rational polynomial expression. The two-sided projection conditions (Petro-Galerkin condition) are:

\[
x_b \in \text{CK}(A, b, k_b, m_b), & \quad r_b = b - (zI - A)x_b \in \text{CK}(A, b, k_b, m_b + 1), \\
s.t. & \quad r_b \bot \text{CK}(A^H, c, k_c, m_c),
\]

(2.17)
and
\[ x_c \in \text{CK}(A^H, c, k_c, m_c), \quad r_c = c - (zI - A)^H x_c \in \text{CK}(A^H, c, k_c, m_c + 1), \]
s.t. \[ r_c \perp \text{CK}(A, b, k_b, m_b). \]

Thus, we get \( \tilde{h}(z) = x^H b = c^H x_b \), where
\[ x_b = \tilde{b} (zI - \tilde{W}^H A \tilde{V})^{-1} \tilde{W}^H b, \quad x_c = \tilde{W} (zI - \tilde{W}^H A \tilde{V})^{-H} \tilde{V}^H c. \]

By (2.15), the rational polynomial expressions are
\[ x_b = \chi_b(A, z)b, \quad \chi_b(\lambda, z) \in \mathbb{P}_{l-1}(\lambda)/\varphi(\lambda), \]
\[ r_b = \gamma_b(A, z)b, \quad \gamma_b(\lambda, z) \in \mathbb{P}_l(\lambda)/\varphi(\lambda). \]

Their relations are given by
\[ r_b = b - (zI - A)x_b, \]
\[ \gamma_b(\lambda, z) = 1 - (z - \lambda)\chi_b(\lambda, z), \]
\[ \chi_b(\lambda, z) = \frac{1 - \gamma_b(\lambda, z)}{z - \lambda}. \] (2.18)

Thus, we still have the constraint condition: \( \gamma_b(z, \lambda) = 1 \).

**2.2.2. The derivation.** We first give the expression of \( r_b \) and \( r_c \).

**Lemma 2.10.** Suppose relations (2.16) hold. Set \( g_b(z) := \Lambda(z)/\varphi(z) \) and \( g_c(z) := \Lambda(z)/\psi(z) \), where \( \Lambda(\lambda) \) is the monic characteristic polynomial of \( \tilde{T}_l = \tilde{W}^H A \tilde{V} \). Then, it holds that
\[ \gamma_b(\lambda, z) = \frac{g_b(\lambda)}{g_b(z)}, \quad r_b = \gamma_b(A, z)b, \]
\[ \gamma_c(\lambda, z) = \frac{g_c(\lambda)}{g_c(z)}, \quad r_c^H = c^H \gamma_c(A, z). \]

**Proof.** Translate (2.17) into the standard Krylov subspace language by (2.15), we obtain
\[ x_b \in \text{Krylov}(A, b, l), \quad r_b = b - (zI - A)x_b \in \text{Krylov}(A, \varphi(A)^{-1}b, l + 1), \]
s.t. \[ r_b \perp \text{Krylov}(A^H, \psi(A)^{-H}c, l). \]

By Lemma 2.3, we directly obtain \( r_b = \rho \Lambda(A)[\varphi(A)^{-1}b] = \rho g_b(A)b \), where \( \Lambda(\lambda) \) is the monic characteristic polynomial of \( \tilde{T}_l \). When \( z \) varies, the coefficient \( \rho \) changes. So, we can consider \( \rho \) as a function with respect to the variable \( z \). After we use a new notation \( \rho(z) \), we obtain
\[ \gamma_b(\lambda, z) = \rho(z) \frac{\Lambda(\lambda)}{\varphi(\lambda)} = \rho(z) g_b(\lambda). \]

Because the constraint condition \( \gamma_b(z, \lambda) = 1 \), we obtain \( \rho(z) = 1/g_b(z) \). Hence, \( \gamma_b(\lambda, z) = g_b(\lambda)/g_b(z) \). Similarly, we shall obtain the result about \( r_c \). □

**Remark 2.11.** By relation (2.18), we obtain a new expression of \( \tilde{h}(z) = c^H x_b = x_b^H b \):
\[ \hat{h}(z) = c^H \chi_b(A, z)b = c^H \chi_c(A, z)b, \]
\[ \chi_b(\lambda, z) = \frac{1 - \gamma_b(\lambda, z)}{z - \lambda}, \quad \chi_c(\lambda, z) = \frac{1 - \gamma_c(\lambda, z)}{z - \lambda}. \]
Theorem 2.12. Suppose the Lanczos biorthogonalization procedure of \([A, \varphi(A)^{-1}b, \psi(A)^{-H}c]\) does not break out until \((l+1)\)th iteration. The formed matrices satisfy (2.16). Then, it holds that
\[
h(z) - \hat{h}(z) = c^H(zI - A)^{-1}b - c^H\hat{V}(zI - \hat{W}H\hat{A}\hat{V})^{-1}\hat{W}Hb
= r_c^H(zI - A)^{-1}r_b
= \frac{1}{g_b(z)g_c(z)}c^Hg_c(A)(zI - A)^{-1}g_b(A)b,
\]
where \(\Lambda(\lambda)\) is the monic characteristic polynomial of \(\tilde{T}_l = \hat{W}H\hat{A}\hat{V}\).

The proof is straightforward by our substituting the result of Lemma 2.10 into \(e(z) = r_c^H(zI - A)^{-1}r_b\). The assumption \(c^H\psi(A)^{-1}\varphi(A)^{-1}b = 1\) in (2.16) also does not influence the result. The discussion is almost the same as the one about \(c^Hb = 1\) for Theorem 2.5, which is stated in Remark 2.6. In a word, we obtain the error formula by using special bases \(\hat{V}\) and \(\hat{W}\) of general subspaces CK(A, b, k_b, m_b) and CK(A^H, c, k_c, m_c).

2.2.3. Explanation of the error from Gauss quadrature. We give another proof of Theorem 2.12 from the viewpoint of Gauss quadrature, like what we do in Section 2.1.3 for Theorem 2.5.

Proposition 2.13. Suppose (2.16) hold. Then, it holds that \(c^H\psi(A)^{-1}P(A)\varphi(A)^{-1}b = c^H\hat{P}(\hat{T}_l)e_1\) for any \(P(\lambda) \in \mathbb{P}_{2l-1}\).

Proof. By (2.16), the relating matrices are formed by Lanczos biorthogonalization procedure of \(A, \varphi(A)^{-1}b\) and \(\psi(A)^{-H}c\). Thus, the proof ends by directly applying Proposition 2.7 onto \(A, \varphi(A)^{-1}b\) and \(\psi(A)^{-H}c\). If \(\varphi(\lambda) = \psi(\lambda) = 1\) (i.e. \(k_b = k_c = 0\)), then the result is actually Proposition 2.7 ( [24, Theorem 2]).

Proposition 2.14. Suppose relations (2.16) hold. Then, it holds that \(c^HQ(A)b = c^H\hat{V}\hat{Q}(\hat{W}H\hat{A}\hat{V})\hat{W}Hb\) for any \(Q(\lambda) \in \mathbb{P}_{2l-1}(\lambda)\hat{W}^\dagger(\lambda)\).

Proof. Similar to Lemma 2.2, for \(\hat{\tau}_l^b(\lambda) := \hat{\alpha}_l^0\lambda^j + \cdots + \hat{\alpha}_l^1\lambda + \hat{\alpha}_l^0\), we obtain
\[
\hat{\tau}_j(A)\varphi(A)^{-1}b = \hat{V}_l\hat{\tau}_j(\hat{T}_l)e_1, \quad j < l
\]
\[
\hat{\tau}_l(A)\varphi(A)^{-1}b = \hat{V}_l\hat{\tau}_l(\hat{T}_l)e_1 + \hat{\alpha}_l^1\hat{\gamma}_l\hat{\gamma}_{l+1}, \quad j = l
\]
\[
\hat{\gamma}_l := \gamma_{l+1} \cdots \gamma_{3}\gamma_2.
\]

Setting \(\hat{\tau}_j(\lambda) = \varphi_{k_b}(\lambda)\), we obtain
\[
\begin{cases}
\varphi_{k_b}(A)\varphi_{k_b}(A)^{-1}b = \hat{V}_l\varphi(\hat{T}_l)e_1, & k_b < l \\
\varphi_{k_b}(A)\varphi_{k_b}(A)^{-1}b = \hat{V}_l\varphi(\hat{T}_l)e_1 + \hat{\alpha}_l\hat{\gamma}_l\hat{\gamma}_{l+1}, & k_b = l, m_b = 0
\end{cases}
\]

Note that \(\hat{W}_l\hat{V}_l = I, \hat{W}_l\hat{V}_{l+1} = 0\) and \(W^H\varphi(A)^{-1}b = e_1\). No matter whether \((k_b < l)\) is true, we obtain
\[
\hat{W}Hb = \hat{W}H\varphi(A)\varphi(A)^{-1}b = \varphi(\hat{T}_l)e_1 = \varphi(\hat{T}_l)\hat{W}H\varphi(A)^{-1}b,
\]
\[
\varphi(\hat{T}_l)^{-1}\hat{W}Hb = \hat{W}H\varphi(A)^{-1}b = e_1. \tag{2.19}
\]

Similarly, we obtain
\[
e_1 = \psi(\tilde{K}_l)^{-1}\hat{V}Hc, \quad c_1^H = c^H\hat{V}\psi(\tilde{K}_l)^{-H} = c^H\hat{V}\psi(\tilde{K}_l)^{-1}. \tag{2.20}
\]

The proof ends by rewriting Proposition 2.13 with (2.19) and (2.20). \(\Box\)

Now, we start to explain the error formula. For simple presentation, we assume that \(\tilde{m}_0 = 1\), where \(\tilde{m}_0 := c^H\psi(A)^{-1}\varphi(A)^{-1}b\). If \(\tilde{m}_0 \neq 1\), then a similar discussion of Remark 2.6 can be applied. We define the linear functional with a weighted term:
\[
\widetilde{\Gamma}(\mathcal{F}) := c^H\psi(A)^{-1}\mathcal{F}(A)\varphi(A)^{-1}b. \tag{2.21}
\]
With the bases from (2.16), we have the Gauss-Christoffel quadrature formula:

\[ \tilde{\mathbf{f}}(\mathcal{F}) = \tilde{\mathbf{f}}_G(\mathcal{F}) + \tilde{\mathbf{e}}(\mathcal{F}), \]

i.e.,

\[ e^H(A)^{-1}F(A)\varphi(A)^{-1}b = e_1^Hf(\tilde{T}_1)e_1 + \tilde{\mathbf{f}}([\Lambda(\lambda)]^2F[\lambda_1, \lambda_2, \lambda_2, \ldots, \lambda_l, \lambda_l, \lambda]). \]  

(2.22)

By Theorem 2.13, we observe that \( \tilde{\mathbf{f}}(\mathcal{P}) = \tilde{\mathbf{f}}_G(\mathcal{P}) \) holds for any \( \mathcal{P}(\lambda) \in \mathbb{F}_{-l-1} \). Thus, we know \( \tilde{\mathbf{f}}_G(\mathcal{F}) = e_1^Hf(\tilde{T}_1)e_1 \) is the Gauss-Christoffel quadrature formula.

Then, we shall proceed the research with the function \( \tilde{\mathcal{H}}(\lambda, z) = \varphi(\lambda)\psi(\lambda)/(z - \lambda) \). After substituting \( \tilde{\mathcal{H}}(\lambda, z) \) into \( \mathcal{F}(\lambda) \) in (2.22), we shall obtain

\[ e^H(zI - A)^{-1}b = e_1^H[\tilde{T}_1](zI - \tilde{T}_1)^{-1}\varphi(\tilde{T}_1)e_1 + \tilde{\mathbf{e}}(\tilde{\mathcal{H}}) = e^H(zI - \hat{\mathbf{W}}^H\hat{\mathbf{V}})^{-1}\hat{\mathbf{W}}^Hb + \tilde{\mathbf{e}}(\tilde{\mathcal{H}}), \]

Note that \( \varphi(\tilde{T}_1)e_1 = \hat{\mathbf{W}}^Hb \) and \( e_1^H[\tilde{T}_1] = e^H\hat{\mathbf{V}} \) are already stated in (2.19) and (2.20). Hence,

\[ e(z) = h(z) - \tilde{h}(z) = \tilde{\mathbf{e}}(\tilde{\mathcal{H}}) = \tilde{\mathbf{f}}([\Lambda(\lambda)]^2H[\lambda_1, \lambda_2, \lambda_2, \ldots, \lambda_l, \lambda_l, \lambda]). \]  

(2.23)

**Lemma 2.15.** Set \( \hat{\mathcal{M}}(\lambda) = [\prod_{i=1}^{n}(\lambda - t_i)]/(z - \lambda) \). For distinct \( \lambda_i (i = 1, 2, \ldots, m) \) with \( m \geq (n + 1) \), it holds that \( \hat{\mathcal{M}}[\lambda_1, \lambda_2, \lambda_3, \ldots, \lambda_m] = [\prod_{i=1}^{n}(z - t_i)]/[\prod_{i=1}^{n}(z - \lambda_i)] \).

**Proof.** Separate every factor in the numerator of \( \hat{\mathcal{M}}(\lambda) \) as \( (\lambda - t_i) = (\lambda - z) + (z - t_i) \) and expand the product. Then, we obtain

\[ \hat{\mathcal{M}}(\lambda) = -(\lambda - z)^{n-1} + a_{n-2}(\lambda - z)^{n-2} + \ldots + a_1(\lambda - z) + a_0 + \frac{\prod_{i=1}^{n}(z - t_i)}{\mathcal{R}(\lambda)}, \]

where \( a_0, a_1, \ldots, a_{n-2} \) are independent of \( \lambda \).

The term \( \mathcal{P}_{n-1}[\lambda_1, \lambda_2, \ldots, \lambda_m] \) is the coefficient of the highest degree term from the interpolating polynomial. Now, the interpolating polynomial is of \( (m - 1) \) degree, while the interpolating polynomial \( \mathcal{P}_{n-1}(\lambda) \) is only of \( (n - 1) \) degree. If the condition \( m \geq n \) holds, then the interpolating polynomial happens to be \( \mathcal{P}_{n-1}(\lambda) \). Thus, we obtain \( \mathcal{P}_{n-1}[\lambda_1, \lambda_2, \lambda_3, \ldots, \lambda_m] = 0 \) from \( m \geq (n + 1) \).

Here, we do not use the well known relation between the divided differences and the high order derivatives (e.g. [13, Exercise 3.3.20]). The reason is described in Remark 2.8. Otherwise, we directly obtain

\[ \mathcal{P}_{n-1}[\lambda_1, \lambda_2, \ldots, \lambda_m] = \mathcal{P}_{n-1}(m-1)(\xi)/[(m-1)!] = 0. \]

The numerator of \( \mathcal{R}(\lambda) \) is independent of \( \lambda \). So, we can consider \( \mathcal{R}(\lambda) \)'s numerator as a coefficient. Together it with Lemma 2.9, we obtain \( \mathcal{R}[\lambda_1, \lambda_2, \ldots, \lambda_m] = [\prod_{i=1}^{n}(z - t_i)]/[\prod_{i=1}^{n}(z - \lambda_i)] \). Thus, the proof ends by noticing \( \hat{\mathcal{M}}[\lambda_1, \lambda_2, \lambda_3, \ldots, \lambda_m] = \mathcal{P}_{n-1}[\lambda_1, \lambda_2, \lambda_3, \ldots, \lambda_m] + \mathcal{R}[\lambda_1, \lambda_2, \ldots, \lambda_m]. \)

For \( \hat{\mathcal{H}}(\lambda, z) = \varphi(\lambda)\psi(\lambda)/(z - \lambda) \), by Lemma 2.15, we can easily get

\[ \hat{\mathcal{H}}[\lambda_1, \lambda_2, \lambda_2, \ldots, \lambda_l, \lambda] = \left\{ \frac{\varphi(z)\psi(z)}{[\Lambda(z)]^2} \right\} z - \lambda, \]  

(2.24)

Substitute (2.24) into (2.23), use definition (2.21) and notice that the term in large braces is independent of \( \lambda \). Then, we shall obtain an expression of \( e(z) \) which is the same as the result of Theorem 2.12.

In conclusion, we use a weighted linear functional (2.22) for the function \( \hat{\mathcal{H}}(\lambda, z) = \varphi(\lambda)\psi(\lambda)/(z - \lambda) \). The error formula is the Gauss quadrature remainder, when the Gauss quadrature (2.22) is applied onto \( \hat{\mathcal{H}}(\lambda, z) \).

The difference between Section 2.1.3 and here is that we use different weight terms for the linear functionals. Thus, the shifts \( t_i, s_i \) in \( \varphi(\lambda), \psi(\lambda) \) change the linear functional from (2.10) to (2.22), like the role of the
preconditioner $M$ in Preconditioned Conjugate Gradient (PCG) method. [60, Section 9.2] clearly reveals how $M$ changes the inner product in PCG.

Next, we provide the common form of Gauss quadrature, which is used in Section 2.4.2.

Remark 2.16. To give a simple expression, we assume $\lambda_i(i = 1, 2, \ldots, l)$ are distinct here. Otherwise, the Gauss quadrature formula includes higher order derivates terms [56, Section 6].

Let $\mathcal{L}_i(\lambda)$ be the Lagrange basis functions on the nodes $\lambda_i$:

$$\hat{\mathcal{L}}_i(\lambda) = \prod_{j=1, j \neq i}^{l} \frac{\lambda - \lambda_j}{\lambda_i - \lambda_j}. \tag{2.25}$$

Then, the Lagrange interpolating polynomial of $\hat{\mathcal{H}}(\lambda, z) = \varphi(\lambda)\psi(\lambda)/(z - \lambda)$ is $\hat{P}_{l-1}(\lambda) = \sum_{i=1}^{l} \hat{H}(\lambda_i)\hat{\mathcal{L}}_i(\lambda)$.

Hence, $\tilde{h}(z) = e^{H} \hat{\mathcal{V}}(zI - \hat{W}^H \hat{A}^H)^{-1}\hat{W}^H b = e^{H} \hat{R}(zS^H \hat{W}^H \hat{V}R - S^H \hat{W}^H \hat{A}^H \hat{V}R)^{-1}S^H \hat{W}^H b$

$$= e^{H} \hat{V}(zW^H \hat{V} - \hat{W}^H \hat{A}^H)^{-1}\hat{W}^H b = e^{H} \hat{V}(zI - \hat{W}^H \hat{A}^H)^{-1}\hat{W}^H b.$$

By Theorem 2.5, we obtain

$$h(z) - \tilde{h}(z) = \frac{1}{g_b(z)g_c(z)}e^{H}g_c(A)(zI - A)^{-1}g_b(A)b,$$

where $\lambda_i$ are eigenvalues of $\hat{W}^H \hat{A}^H \hat{V}$. In this formula, the only thing related to the bases $\hat{V}$ and $\hat{W}$ are the eigenvalues. Let us see how to relate these eigenvalues to the bases $V$ and $W$. Obviously, we have $\text{eig}(W^H A \hat{V}) = \text{eig}(S^{-1}W^H A R) = \text{eig}((SR)^{-1}W^H A V) = \text{eig}((W^H V)^{-1}W^H A V).$ $\square$

Researchers already use rational biorthogonal basis to design MOR [5,6,22,23]. Since the error formula is independent of the bases, we obviously prefer $V$ and $W$ to be orthonormal in practical implementation. That is $V_i^H V_i = I$, $W_i^H W_i = I$ and $W_i^H V_i \neq I$, where span$(V_i) = \text{CK}(A,b,k_b,m_b)$ and span$(W_i) = \text{CK}(A^H,c,k_c,m_c)$.

To obtain the orthonormal bases we can apply Arnoldi-like procedure onto the basis (2.1). If the shifts sets $T$ and $S$ are given, then a more convenient approach is to call A Rational Krylov Toolbox for MATLAB [12].

For $s_i \neq s_j$, it holds that

$$[(\lambda - s_i)^{-1}, (\lambda - s_j)^{-1}] \begin{bmatrix} 1 & (s_i - s_j)^{-1} \\ 0 & 1 \end{bmatrix} = [(\lambda - s_i)^{-1}, (\lambda - s_i)^{-1}(\lambda - s_j)^{-1}] .$$

Thus, for distinct shifts $s_i$, we can obtain the orthonormal basis by orthogonalizing $[(A - s_1 I)^{-1}b, (A - s_2 I)^{-1}b, \ldots]$. It is more convenient than our orthogonalizing $[(A - s_1 I)^{-1}b, (A - s_2 I)^{-1}(A - s_1 I)^{-1}b, \ldots]$ before.

Use new notation:

$$G_{\text{two}}(\lambda) := g_b(\lambda)g_c(\lambda) = \frac{\Lambda(\lambda) \Lambda(\lambda)}{\varphi(\lambda) \psi(\lambda)}, \tag{2.26}$$

the error formula is simplified as

$$e(z) = h(z) - \tilde{h}(z) = \frac{1}{G_{\text{two}}(z)}e^{H}(zI - A)^{-1}G_{\text{two}}(A)b. \tag{2.27}$$
2.4. The MOR error is the remainder of the Hermitian formula. Hermitian formula is the Cauchy integral form of the interpolation remainder [43, (8)] [26, Page 59]. After transforming the polynomial to the rational polynomial [36, Page 33], we are able to obtain an error formula of rational polynomial interpolation, which is named as Walsh-Hermite formula in [37, Page 19].

**Lemma 2.17.** (Hermite) Suppose the boundary $\Gamma$ of $\Sigma$ consists of finitely many rectifiable Jordan curves with positive orientation relative to $\Sigma$, and suppose $M(z)$ is analytic in $\Sigma$ and continuous in $\Sigma \cup \Gamma$. Suppose the interpolation conditions hold, i.e., $M(\alpha_i) = P_{k-1}(\alpha_i)$ for $\alpha_i \in \Sigma(i = 1, 2, \ldots, k)$. Write $\pi_k^\alpha(z) = \prod_{i=1}^k (z - \alpha_i)$. Then, it holds that

$$M(z) - P_{k-1}(z) = \frac{1}{2\pi i} \oint_{\Gamma} \frac{\pi_k^\alpha(z) M(\zeta)}{\zeta - z} d\zeta.$$  

**Lemma 2.18.** (Walsh-Hermite) Let $Q_{k-1,k}(z) \in Q_{k-1,k}(z)$ be a rational interpolating polynomial of $N(z)$ with poles $\beta_i$ and interpolating nodes $\alpha_i$. Write

$$G_k^{\alpha,\beta}(z) := \prod_{i=1}^k \frac{z - \alpha_i}{z - \beta_i} = \frac{(z - \alpha_1)(z - \alpha_2) \cdots (z - \alpha_k)}{(z - \beta_1)(z - \beta_2) \cdots (z - \beta_k)}.$$

Suppose the boundary $\Gamma$ of $\Sigma$ consists of finitely many rectifiable Jordan curves with positive orientation relative to $\Sigma$, and suppose $N(z)$ is analytic in $\Sigma$ and continuous in $\Sigma \cup \Gamma$. If interpolating nodes $\alpha_i$ are in $\Sigma$, then it holds that

$$N(z) - Q_{k-1,k}(z) = \frac{1}{2\pi i} \oint_{\Gamma} \frac{G_k^{\alpha,\beta}(z) N(\zeta)}{\zeta - z} d\zeta.$$  

**Proof.** Let $\pi_k^\alpha(z) := \prod_{i=1}^k (z - \beta_i)$, $N(z) := N(z)\pi_k^\alpha(z)$ and $P_{k-1}(z) := Q_{k-1,k}(z)\pi_k^\alpha(z)$. By the rational interpolation condition, we obtain $N(\alpha_i) = P_{k-1}(\alpha_i)$ for $\alpha_i \in \Sigma(i = 1, 2, \ldots, k)$. Thus, Lemma 2.17 is applied.

$$N(z)\pi_k^\alpha(z) - P_{k-1}(z) = N(z) - P_{k-1}(z) = \frac{1}{2\pi i} \oint_{\Gamma} \frac{\pi_k^\alpha(z) N(\zeta)}{\zeta - z} d\zeta = \frac{1}{2\pi i} \oint_{\Gamma} \frac{\pi_k^\alpha(z) N(\zeta)\pi_k^\alpha(\zeta)}{\zeta - z} d\zeta. \quad (2.28)$$

The proof is completed after our dividing (2.28) by $\pi_k^\alpha(z)$. \qed

In the next two subsections, we apply Lemma 2.18 onto the resolvent function $H(\lambda, z) = 1/(z - \lambda)$ with respect to variables $z$ and $\lambda$, respectively. Note the interpolation nodes and poles of these two cases are opposite. The key step in the two proofs is the interchange of the problem resolvent function $H(\lambda, z)$ and the resolvent function in the Cauchy integral. Therefore, if other problems do not have the resolvent function term inside, we may not expect to acquire an explicit error formula.

### 2.4.1. Variable $z$

To make use of Lemma 2.18, we substitute $h(z) \in Q_{n-1,n}(z)$ and $\hat{h}(z) \in Q_{l-1,l}(z)$ into $N(z)$ and $Q_{k-1,k}(z)$, respectively. For simplicity, we assume $k_b = k_c = l$ and all of the shifts $t_i, s_i$ (from $\varphi(\lambda), \psi(\lambda)$) are finite. Suppose there exist a region $\Sigma$ satisfying $\text{eig}(A) \cup \{\lambda_i\} \subseteq \Sigma$ and $\{s_i, t_i\} \subseteq \Sigma^-$. Now, we know $\hat{h}(z)$ is a rational interpolating polynomial of $h(z)$ with poles $\lambda_i$ (doubled) and interpolating nodes $t_i, s_i$. Thus, we substitute $G_k^{\alpha,\beta}(z) = 1/G_{\text{two}}(z)$ into Lemma 2.18, where $G_{\text{two}}(z)$ is from (2.26). It is easy to check that $\hat{h}(z)$ is analytic on the $\Sigma^-$. By Lemma 2.18, for $z \in \Sigma^-$, it holds that

$$h(z) - \hat{h}(z) = \frac{1}{2\pi i} \oint_{\Gamma} \frac{G_k^{\alpha,\beta}(z) h(\zeta)}{G_k^{\alpha,\beta}(\zeta) \zeta - z} d\zeta = \frac{1}{2\pi i} \oint_{\Gamma} \frac{G_{\text{two}}(\zeta) e^H(\zeta I - A)^{-1} b}{\zeta - z} d\zeta$$

$$= \frac{1}{G_{\text{two}}(z)} \frac{1}{2\pi i} e^H \left[ \oint_{\Gamma} \frac{G_{\text{two}}(\zeta)}{\zeta - z} (\zeta I - A)^{-1} d\zeta \right] b$$

$$= \frac{1}{G_{\text{two}}(z)} \frac{1}{2\pi i} e^H G_{\text{two}}(A) (z I - A)^{-1} b.$$
At the last equality, we use the Cauchy integral definition for function of matrices (e.g. [38, Definition 1.11]), since $G_{two}(\zeta)/(z - \zeta)$ with respect to $\zeta$ is analytic on $\Sigma \supseteq \text{eig}(A) \cup \{\lambda_i\}$.

### 2.4.2. Variable $\lambda$

This explanation is closely related to the first explanation which uses the Gauss quadrature. We substitute $\tilde{H}(\lambda) = \varphi(\lambda)\psi(\lambda)/(z - \lambda)$ into $\tilde{N}(z)$ in the proof of Lemma 2.18. Now, the involving variable is $\lambda$. For simplicity, we assume there exist a set $\Sigma$ satisfying $\text{eig}(A) \cup \{\lambda_i\} \subseteq \Sigma$ and $\{s_i, t_i\} \subseteq \Sigma^-$. To have a simple interpolating polynomial expression, we assume all of $\{\lambda_i\}$ are distinct.

Let $\tilde{P}_{2l-1}(\lambda) \in \mathbb{P}_{2l-1}(\lambda)$ be the Hermitian interpolating polynomial of $\tilde{H}(\lambda)$ on interpolating nodes $\lambda_i$ (doubled). Its explicit expression is well known (e.g. [13, Theorem 3.9]).

\[
\tilde{H}(\lambda_i) = \tilde{P}_{2l-1}(\lambda_i), \quad \tilde{H}'(\lambda_i) = \tilde{P}'_{2l-1}(\lambda_i), \quad i = 1, 2, \ldots, l
\]

\[
\tilde{P}_{2l-1}(\lambda) = \sum_{i=1}^{l} \tilde{H}(\lambda_i) \{\tilde{L}_i^2(\lambda)(1 - 2(\lambda - \lambda_i)) \tilde{L}_i(\lambda)\} + \sum_{i=1}^{l} \tilde{H}'(\lambda_i) [(\lambda - \lambda_i) \tilde{L}_i^2(\lambda)], \quad (2.29)
\]

where $\tilde{L}_i(\lambda)$ is the Lagrange basis function polynomial (2.25). By Lemma 2.17, we obtain

\[
\tilde{H}(\lambda) - \tilde{P}_{2l-1}(\lambda) = \frac{1}{2\pi i} \int_{\Gamma} \frac{[A(\lambda)]^2}{[A(\zeta)]^2} \frac{\tilde{H}(\zeta)}{\zeta - \lambda} d\zeta = \frac{1}{2\pi i} \int_{\Gamma} \frac{\varphi(\zeta)\psi(\zeta)}{z - \zeta} \frac{1}{\zeta - \lambda} d\zeta
\]

\[
= \frac{[A(\lambda)]^2}{2\pi i} \int_{\Gamma} \frac{1}{[A(\zeta)]^2} \frac{\varphi(\zeta)\psi(\zeta)}{\zeta - \lambda} \frac{1}{\zeta - z} d\zeta
\]

\[
= \frac{[A(\lambda)]^2}{2\pi i} \int_{\Gamma^+} \left\{ \frac{1}{[A(\zeta)]^2} \frac{\varphi(\zeta)\psi(\zeta)}{\zeta - \lambda} \right\} \frac{1}{\zeta - z} d\zeta = \frac{[A(\lambda)]^2}{[A(\zeta)]^2} \frac{\varphi(z)\psi(z)}{z - \lambda}.
\]

Cauchy integral formula is used at last equality, since the function in braces with respect to $\zeta$ is analytic on $\Sigma^-$. This remainder formula is a quantity equality, which can be proved by other ways. Actually, we have

\[
\tilde{H}(\lambda) - \tilde{P}_{2l-1}(\lambda) = \tilde{H}[\lambda_1, \lambda_1, \lambda_2, \lambda_2, \ldots, \lambda_l, \lambda_l, \lambda][A(\lambda)]^2,
\]

(2.31)

where $\tilde{H}[\lambda_1, \lambda_1, \lambda_2, \lambda_2, \ldots, \lambda_l, \lambda_l, \lambda]$ is discussed in (2.24).

To obtain the expression of $e(z)$, we now have two approaches: 1. Directly apply the linear functional with a weighted term (2.21) onto (2.31). 2. Divide (2.31) by $\varphi(\lambda)\psi(\lambda)$, and then use the linear functional (2.10).

Finally, we answer the question: How does $e^H\psi(A)^{-1}P_{2l-1}(A)\varphi(A)^{-1}b$ become to $\tilde{h}(z) = e^H\tilde{V}(zI - \tilde{W}^H\tilde{A})^{-1}\tilde{W}^Hb$? By Proposition 2.14, we obtain $e^H\psi(A)^{-1}P_{2l-1}(A)\varphi(A)^{-1}b = e^H\tilde{V}P_{2l-1}(\tilde{W}^H\tilde{A})\tilde{W}^Hb$. In (2.29), the term $[(\lambda - \lambda_i)\tilde{L}_i^2(\lambda)]$ obviously has the factor $A(\lambda)$ in its numerator. By Cayley-Hamilton theorem, these terms becomes zero, when we put $\tilde{T} = \tilde{W}^H\tilde{A}\tilde{V}$ inside. Thus, we obtain $\tilde{P}_{2l-1}(\tilde{T}) = \tilde{P}_{l-1}(\tilde{T})$, where $\tilde{P}_{l-1}(\lambda)$ only needs to satisfy the interpolation condition: $\tilde{H}(\lambda_i) = \tilde{P}_{l-1}(\lambda_i), i = 1, 2, \ldots, l$. Actually, we have discussed this $\tilde{P}_{l-1}(\lambda)$ in Remark 2.16.

In conclusion, the relation between the third (this subsection) and first explanation (Section 2.2.3) is the same as the one between interpolation polynomial theory and Gauss quadrature theory. The latter is well known.

### 2.5. The remainder formula of the descriptor model: $E \neq I$

We discuss how $h(z) = e^H(zE - A)^{-1}b$ is approximated by $\hat{h}(z) = e^H[V(z\tilde{W}^H\tilde{E}V - \tilde{W}^H\tilde{A}V)^{-1}\tilde{W}^Hb$. Obviously, we have $h(z) = e^H[zI - (E^{-1}A)]^{-1}(E^{-1}b)$. Substituting it into Theorem 2.1, we obtain the error formula of the descriptor model.

\[
\hat{h}(z) = e^H[V(z\tilde{W}^H\tilde{E}V - \tilde{W}^H\tilde{A}V)^{-1}\tilde{W}^H(E^{-1}b)]
\]

\[
= e^H[V(zE^{-1}H\tilde{E}V - (E^{-1}H\tilde{A}V)^{-1}(E^{-1}H\tilde{W})^Hb]
\]

\[
= e^H[V(z\tilde{W}^H\tilde{E}V - \tilde{W}^H\tilde{A}V)^{-1}\tilde{W}^Hb,
\]
where $\mathcal{V}$ and $\widetilde{\mathcal{W}}$ are set up by $(E^{-1}A,E^{-1}b,c)$ in Theorem 2.1. Actually, we use $\mathcal{W} = E^{-H}\widetilde{\mathcal{W}}$ instead of $\widetilde{\mathcal{W}}$.

**Theorem 2.19.** Let $\text{span}(\mathcal{V}) = \text{CK}(E^{-1}A,E^{-1}b,k_b,m_b)$ and $\text{span}(\mathcal{W}) = \text{CK}((AE^{-1})^H,E^{-H}c,k_c,m_c)$ with $k_b + m_b = k_c + m_c =: l$. Suppose that the Lanczos biorthogonalization procedure of $A$, $[\prod_{j=2}^{k_b}(A - s_jE)^{-1}E][A - s_1E]^{-1}b$ and $\prod_{j=2}^{k_c}(A - t_jE)^{-H}E^H[A - t_1E]^{-H}c$ does not break until $(l + 1)$th iteration. With notations (2.2) and (2.3), we have

$$
e(z) = h(z) - \hat{h}(z) = c^H(zE - A)^{-1}b - c^H\mathcal{V}(zW^HEV - W^HAV)^{-1}W^Hb$$

$$= \frac{1}{g_b(z)g_c(z)}c^Hg_c(E^{-1}A)(zI - E^{-1}A)^{-1}g_b(E^{-1}A)E^{-1}b$$

$$= \frac{1}{g_b(z)g_c(z)}c^Hg_c(E^{-1}A)g_b(E^{-1}A)(zE - A)^{-1}b,$$

(3.2)

where $\Delta(\lambda)$ is the monic characteristic polynomial of $(W^HEV)^{-1}W^HAV$.

**3. One-sided Galerkin projection.** Obviously, we can use known methods to approximate $\mathcal{H}(A)b$. It is a function of matrices, which is studied in [38, Chapter 13] and [36,37,39]. After pre-multiplying it by $c^H$, we shall obtain an approximation of the transfer function. The basis is obtained by

$$\text{CK}(E^{-1}A,E^{-1}b,k,m) : = \text{RK}(E^{-1}A,E^{-1}b,S,k) \cup \text{Krylov}(E^{-1}A,E^{-1}b,m),$$

$$\text{span}(V_{2l}) = \text{CK}(E^{-1}A,E^{-1}b,k,m) = \text{Krylov}(E^{-1}A,\varphi_k(E^{-1}A)^{-1}E^{-1}b,2l),$$

$$V^HV = I, \quad \varphi_k(\lambda) = \prod_{j=1}^{k}(\lambda - s_j), \quad k + m = 2l.$$  

(3.1)

By summarizing [9, (2.1)] and [19, (2.2)], we obtain the error of one-sided projection method.

**Theorem 3.1.** Suppose the dimension of $\text{CK}(E^{-1}A,E^{-1}b,k,m)$ is $2l$. With notations by (3.1), we have

$$h(z) - \hat{h}(z) = c^H(zE - A)^{-1}b - c^HV(zV^HEV - V^HAV)^{-1}V^Hb$$

$$= \frac{1}{G_{\text{one}}(z)}c^HG_{\text{one}}(E^{-1}A)(zE - A)^{-1}b,$$

where

$$G_{\text{one}}(\lambda) := \frac{\Lambda_{\text{one}}(\lambda)}{\varphi(\lambda)},$$

(3.2)

with $\Lambda_{\text{one}}(\lambda) = \prod_{i=1}^{2l}(\lambda - \lambda_i)$ be the monic characteristic polynomial of $(V^HEV)^{-1}V^HAV$.

We observe $G_{\text{one}}(\lambda)$ has the similar form like (2.26) in the two-sided projection. The main difference is that: the order of the reduced system by the two-sided projection is $l$, while the one-sided projection gets $2l$. In comparison to the numerical quadrature, it is quite comprehensible. To acquire higher degree of accuracy, one approach is to use Gauss quadrature (two-sided projection method, cf. Section 2.2.3), while another approach is to use higher interpolating polynomials (one-sided projection method).

**4. Interpolatory $H_\infty$ norm MOR.** In this section, we suppose $A$ is $c$-stable, i.e., $\text{eig}(A)$ are on left half plane. Norm $\parallel \cdot \parallel_{H_\infty}$ is defined in a $\mathcal{H}_\infty$-space. The space requires the function matrix is analytic and bounded in the open right hand half plane. With $h(z) = c(zI - A)^{-1}b$, we have $\parallel h \parallel_{H_\infty} = \sup_{z \in \mathbb{C} \cup \{\infty\}} |c^H(zI - A)^{-1}b|$. MOR in $H_\infty$ norm sense is to solve

$$\parallel h(z) - \hat{h}_s(z) \parallel_{H_\infty} = \min_{\dim(h) = l} \parallel h(z) - \hat{h}(z) \parallel_{H_\infty},$$

(4.1)

where $h(z) = c^H(zE - A)^{-1}b$,

$$\hat{h}(z) = c^H_t(zE_t - A_t)^{-1}b_t + d_t.$$ 

(4.2)
Thus, we get \( \lim_{l \to \infty} \) from Section with a constant norm estimation of the model error by using the Hankel singular values \( k \). Thus, we set \( k = k_c = l \). In conclusion, we shall discuss the following problem:

\[
\min_{s_1, s_2, \ldots, s_l, t_1, t_2, \ldots, t_l} \sup_{z \in \mathbb{R}U\{\infty\}} |e(z)| = \min_{s_1, s_2, \ldots, s_l, t_1, t_2, \ldots, t_l} \sup_{z \in \mathbb{R}U\{\infty\}} |h(z) - \tilde{h}(z)|
\]

\[
= \min_{s_1, s_2, \ldots, s_l, t_1, t_2, \ldots, t_l} \sup_{z \in \mathbb{R}U\{\infty\}} \left| \frac{1}{G(z)} \right| |c^H G(E^{-1}A)(zE - A)^{-1}b|,
\]

where \( G(z) \) is either \( G_{\text{two}}(z) \) in (2.26) or \( G_{\text{one}}(z) \) in (3.2).

**Lemma 4.1.** ([36, Theorem 4.9]) Let \( f \) be analytic in a neighborhood of \( \mathcal{H}(A) \), and let \( \Sigma \supseteq \mathcal{H}(A) \). There holds \( \|f(A)\| \leq C\|f\|_{\Sigma} \) with a constant \( C \leq 11.08 \).

For \( \mathcal{H}(E^{-1}A) \subset \Sigma \), it is easy to check that

\[
|c^H G(E^{-1}A)(zE - A)^{-1}b| \leq \tilde{D} \|G(E^{-1}A)\|_2 \leq \tilde{D} \|G(E^{-1}A)\|_{\Sigma} = \tilde{D} \sup_{\lambda \in \Sigma} |G(\lambda)|.
\]

Thus, problem (4.3) is approximately solved by

\[
\min_{s_1, s_2, \ldots, s_l, t_1, t_2, \ldots, t_l} \sup_{\lambda \in \Sigma} \frac{|G(\lambda)|}{\inf_{z \in \mathbb{R}U\{\infty\}} |G(z)|}.
\]

### 4.1. Logarithmic potential theory and asymptotically optimal shifts.

The problem (4.4) is closely related to the generalized Zolotaryov problem [37, (17)], which can be solved by logarithmic potential theory [66, Chapter 12]. Güttd's PhD thesis work [36, 37] clearly states how to handle this type problem in a more general setting. We give quite short description here.

We abbreviate \( \mathcal{H}(\lambda, z) = 1/(z - \lambda) \) to \( \mathcal{H}(\lambda) \). Thus, \( h(z) = c^H \mathcal{H}(A)b \). We use the special bases \( \tilde{W}, \tilde{V} \) from Section 2.2. Thus, \( \tilde{h}(z) = c^H \tilde{V} \mathcal{H}(\tilde{W}^H \tilde{A}^T)\tilde{W}^H b \). We discuss the function \( \mathcal{H}(\lambda) \) on the region \( \Sigma \supseteq \mathcal{H}(A) \cup \mathcal{W}(\tilde{W}^H \tilde{A}^T) \). The counterpart of [36, Lemma 4.6] [37, Lemma 3.1] is Proposition 2.14. Thus, similar to [36, Theorem 4.10] [37, Corollary 3.4], we obtain:

**Proposition 4.2.** (Near-optimality) Suppose relations (2.16) hold. Suppose that \( \mathcal{H}(\lambda) = 1/(z - \lambda) \) is analytic in a neighborhood of a compact set \( \Sigma \supseteq \mathcal{W}(A) \cup \mathcal{W}(\tilde{W}^H \tilde{A}^T) \). Then the approximation \( c^H \tilde{V}(zI - \tilde{W}^H \tilde{A}^T)^{-1}\tilde{W}^H b \) satisfies

\[
|c^H (zI - A)^{-1}b - c^H \tilde{V}(zI - \tilde{W}^H \tilde{A}^T)^{-1}\tilde{W}^H b| \leq C(1 + \|\tilde{V}\|\|\tilde{W}\|b\|c\| \min_{\lambda \in \Sigma} \|\mathcal{H}(\lambda) - \mathcal{Q}(\lambda)\|_{\Sigma})
\]

with a constant \( C \leq 11.08 \).
Proof. By Theorem 2.14, we have $c^HQ(A)b = c^H\hat{V}Q(\hat{W}^HA\hat{V})\hat{W}Hb$ for $Q(\lambda) \in \mathbb{P}_{2\nu-1}(\lambda)$. 

$$|c^H(zI - A)^{-1}b - c^H\hat{V}(zI - \hat{W}^HA\hat{V})^{-1}\hat{W}Hb| = |c^H\mathcal{H}(A)b - c^H\hat{V}\mathcal{H}(\hat{W}^HA\hat{V})\hat{W}Hb|$$

$\leq \|b\| \|c\| (\|\mathcal{H}(A) - Q(A)\| + \|V\| \|\mathcal{H}(\hat{W}^HA\hat{V}) - Q(\hat{W}^HA\hat{V})\||\hat{W}\|)$

$\leq C\|b\| \|c\| (\|\mathcal{H}(\lambda) - Q(\lambda)\|_{\mathcal{W}(A)} + \|\hat{V}\| \|\mathcal{H}(\lambda) - Q(\lambda)\|_{\mathcal{W}(\hat{W}^HA\hat{V})}\||\hat{W}\|)$

$\leq C(1 + \|\hat{V}\| \|\hat{W}\|)|b||c| \|\mathcal{H}(\lambda) - Q(\lambda)\|_{\Sigma}.$

Let the numerator of the $Q(\lambda)$ to be any. Then, we obtain the minimization. \qed

Based an estimation of Hermite-Walsh formula [36, Page 33], by using some special shifts, a bound of $\min Q(\lambda) \in \mathbb{P}_{2\nu-1}(\lambda)/\|\mathcal{W}(\lambda)\|_\Sigma$ can be obtained, see [36, (7.5)] [37, (18)] [43, Theorem 6 (Walsh)]. The obtained shifts are asymptotically optimal shifts and used for forming rational Krylov subspaces. Practical approaches to compute the shifts are discussed in [36, Page 95] [37, Page 12]. Our problem involves the resolvent function $\mathcal{H}(\lambda) = 1/(z - \lambda)$ and a parameter $z$. Some uniform results are summarized in [37, Section 4.1].

This theory is for the approximation of a general function, and is based on an estimation of Walsh-Hermitian formula. However, for our problem, the Cauchy integral in Walsh-Hermitian formula is computed successfully. The term is expressed explicitly when the involving function is the resolvent function (cf. (2.30) and (2.31)). This explicit error formula makes our problem easier.

### 4.2. Approximations of $e(z)$

The full computation of $e(z)$ is expensive, we need some approximations:

**Remark 4.3.** We have these approximations for $|e(z)|$.

$$e(z) = h(z) - \hat{h}(z) = \frac{1}{G(z)}c^HG(E^{-1}A)(zE - A)^{-1}b,$$

**Approximation 1:** $|e(z)| = C_1 \frac{1}{|G(z)|}$

**Approximation 2:** $|e(z)| \leq \frac{1}{|G(z)|} \|c^HG(E^{-1}A)\|_2 \|(zE - A)^{-1}b\|_2$

$\approx C_2 \frac{1}{|G(z)|} \|(zW^HEV - W^HAV)^{-1}W^Hb\|_2,$

**Approximation 3:** $|e(z)| \leq \frac{1}{|G(z)|} \|c^H\|_2 \|G(E^{-1}A)\|_2 \|(zE - A)^{-1}b\|_2$

$\approx C_3 \frac{1}{|G(z)|} \|c^H\|_2 \|(zE - A)^{-1}b\|_2$

$\approx C_3 \frac{1}{|G(z)|} \|c^HV(zW^HEV - W^HAV)^{-1}W^Hb\|.$

The term $G(z)$ is a quantity formula, which implies it can be computed easily. The algorithm in [19] actually utilizes Approximation 1 (cf. Algorithm 1). If all of Ritz values $\lambda_i$ are real, then the constant $C_1$ is closely related to the interpolation remainder, which is expressed by high order derivatives and the unknown $\xi$. The remainder (2.23) and (2.31) are expressed by the divided difference. After turning them into the high order derivatives by (2.12), we shall overwrite the coefficient $C_1$.

Except $1/G(z)$, there is still $z$ in the left of $e(z)$. This means Approximation 1 can be improved. Note that the obtained $s_i$ and $\lambda_i$ are independent of $z$. To approximate $c^HG(E^{-1}A)(zE - A)^{-1}b$, we figure out Approximations 2 and 3, which can be computed in the reduced problems.

To solve problem (4.3), we use a different approach of (4.4) together with the logarithmic potential theory. We actually ignore the term $\|G(E^{-1}A)\|_2$ and pay more attention on $\|(zE - A)^{-1}b\|_2$. The former is independent
Algorithm 1 Adaptive Rational Krylov Subspace Method (ARKSM) [19]

Input: $A, E \in \mathbb{C}^{n \times n}, B \in \mathbb{C}^{n \times m}, C \in \mathbb{C}^{p \times n}$ and $D \in \mathbb{C}^{p \times m}$,

Input: $s_{\min}, s_{\max}, l_{\max}$,

1: $s_1 = s_{\min}, v_1 = (A - s_1 E)^{-1} b$;
2: $s_2 = s_{\max}, v_2 = (A - s_2 E)^{-1} b$;
3: $V = [v_1, v_2]; \quad V = \text{orth}(V)$;
4: for $l = 2, \ldots, l_{\max}$ do
5: \hspace{1em} Update $V^H AV, V^H EV, V^H b$;
6: \hspace{1em} Get Ritz values $\lambda_i \in \text{eig}((V^H EV)^{-1} V^H AV)$;
7: \hspace{1em} Determine $\partial \Xi = \text{convex hull of } \{-\lambda_1, \ldots, -\lambda_l, s_{\min}, s_{\max}\}$;
8: \hspace{1em} Choose the next shift $s_{l+1}$:
9: \hspace{2em} $s_{l+1} = \arg \max_{z \in \partial \Xi} \left| \prod_{j=1}^{l} (z - s_j) / \prod_{j=1}^{l} (z - \lambda_j) \right|$.
10: \hspace{1em} $v_{l+1} = (A - s_{l+1} E)^{-1} b$;
11: \hspace{1em} $V = \text{orth}([V, v_{l+1}])$;
12: end for

Output: $V$; Shifts $s_l(l = 1, 2, \ldots, l_{\max}); \quad \tilde{h}(z) = e^H V (z V^H EV - V^H AV)^{-1} V^H b \approx h(z)$.

of $z$. When the previous shifts are known, the Ritz value are also fixed. We directly consider $\|G(E^{-1} A)\|_2$ as a constant. Meanwhile, in logarithmic potential theory, $\|G(E^{-1} A)\|_2 \approx D \sup_{\lambda \in \Xi} |G(\lambda)|$ is used. In our algorithms, we also consider the influence of $||(z E - A)^{-1} b||_2$. In testing examples, we observe algorithms based on Approximations 2 and 3 have better behavior than the one based on Approximation 1.

In conclusion, the greedy algorithm is used here. The next shifts are obtained by choosing the maximal point of the error. Moreover, we claim that these obtained shifts are distinct, because any obtained shifts satisfies $e(s_j) = 0$, which implies it can not be the maximal point of the error. This implies that we only need to orthogonalize $[V, (A - s_i E)^{-1} v]$ instead of orthogonalizing $[V, (A - s_i E)^{-1} v]$, where $v$ is the last vector of $V$.

5. Greedy algorithms for MOR. Based on different error estimations, there exist many adaptive algorithms for MOR [5,6,22,23,55]. Our algorithm uses the obtained error formula by modifying the algorithm in [19].

5.1. Algorithm ARKSM. In paper [19], the shifts are required to be real numbers or conjugate pairs. For simplicity, we do not have this constrain (See Algorithm 1). The first two shifts are acquired by

\begin{equation}
\begin{aligned}
s_{\min} = \text{eigs}(-A, E, 1, \text{‘sm’}), \quad s_{\max} = \text{eigs}(-A, E, 1, \text{‘lm’}).
\end{aligned}
\end{equation}

Other shifts are selected on the boundary of $\Xi$, where $\Xi$ is a mirror region of Ritz values. If $s_l = -\overline{\lambda}_l$, then we shall get $H_2$ norm optimal MOR [34]. By using the maximal value theorem on $\Xi$, the shifts are picked up on the boundary $\partial \Xi$. Another explanation can be found in [37, Section 4.1].

5.2. Two-sided algorithms. Our greedy two-sided algorithm is Algorithm 2.

Since $E^{-1} A$ is $c$-stable, shifts are selected on right half plane to make $(A - s_i E)$ be nonsingular. The boundary of the right half plane is the image axis. Moreover, we are now doing research on $H_\infty$ norm MOR, which is defined on the image axis. Thus, we shall choose the shifts on the image axis. Choosing shifts on the image axis is not new (e.g. [22,23]). In practice, our shifts are selected on $Z(\alpha, \beta, 500)$, where

\begin{equation}
\begin{aligned}
Z(\alpha, \beta, k) = [-\iota \times \text{logspace}(\alpha, \beta, k), 0, \iota \times \text{logspace}(\alpha, \beta, k)].
\end{aligned}
\end{equation}
Algorithm 2 Two-sided greedy rational Krylov subspace method for MOR

Input: \( A, E \in \mathbb{C}^{n \times n}, B \in \mathbb{C}^{m \times m}, C \in \mathbb{C}^{p \times n} \) and \( D \in \mathbb{C}^{p \times m} \).

Input: \( a, b, k_\text{two}, s_{\text{max}}, l_{\text{max}} \).

1. \( s_1 = |s_{\text{max}}|/10, v_1 = (A - s_1 E)^{-1}b; \)
2. \( t_1 = -|s_{\text{max}}|/10, w_2 = (A - s_2 E)^{-H}C; \)
3. \( V = \text{orth}(v_1); W = \text{orth}(w_1); \)
4. Determine the set for choosing shifts: \( Z_2 = Z(a, b, k_\text{two}) \) from (5.4).
5. for \( l = 1, \ldots, l_{\text{max}} \) do
6. \( \text{Update } W^H AV; W^H EV; W^H b; e^H V; \)
7. \( \text{Get Ritz values } \lambda_i \in \text{eig}((W^H EV)^{-1}W^H AV); \quad \Lambda(z) := \prod_{i=1}^l (z - \lambda_i); \)
8. \( \text{Set new symbols: } \varphi_l(z) := \prod_{i=1}^l (z - s_i); \quad \psi_l(z) := \prod_{i=1}^l (z - t_i); \)
9. \( \text{Choose next shift for } s_{l+1}: \)

\[
\begin{align*}
\text{Option 1 : } & \quad s_{l+1} = \arg \max_{z \in Z_2} \frac{\varphi_l(z) \psi_l(z)}{|\Lambda(z)|^2}, \\
\text{Option 2 : } & \quad s_{l+1} = \arg \max_{z \in Z_2} \frac{\varphi_l(z) \psi_l(z)}{|\Lambda(z)|^2} \| (zW^H EV - W^H AV)^{-1} W^H b \|_2, \quad (5.3) \\
\text{Option 3 : } & \quad s_{l+1} = \arg \max_{z \in Z_2} \frac{\varphi_l(z) \psi_l(z)}{|\Lambda(z)|^2} |c^H V(zW^H EV - W^H AV)^{-1} W^H b|;
\end{align*}
\]

10. Choose the next shift for \( t_{l+1}: \)

\[ t_{l+1} = \text{conj}(s_{l+1}); \]

11. \( v_{l+1} = (A - s_{l+1} E)^{-1}b; w_{l+1} = (A - t_{l+1} E)^{-H}C; \)
12. \( V = \text{orth}(V, v_{l+1}); W = \text{orth}(W, w_{l+1}); \)
13. end for

Output: \( V, W, \quad \hat{h}(z) = c^H V(zW^H EV - W^H AV)^{-1} W^H b \approx h(z). \)

For the two-sided algorithm, \( G(z) \) is \( G_{\text{two}}(z) \) in (2.26). At \( l \)th iteration, shifts \( s_j, t_j (j = 1, 2, \ldots, l) \) are computed. Then, the Ritz values are also acquired. It is important that the variable \( z \) in \( e(z) \) are actually independent of the obtained shifts and Ritz values. Thus, the standard greedy algorithm is quite appropriate to be used here. On Line 9, we provide three options for the next shift, which correspond to the approximations of \( e(z) \) in Remark 4.3. Numerical testing shows Options 2 and 3 behavior better than Option 1.

The computation of (5.3) is not expensive. The computation of \( \varphi_l(z), \psi_l(z) \) and \( \Lambda(z) \) only involves quantity operations. For Options 2 and 3, we need to solve small order linear equations \( (zW^H EV - W^H AV)^{-1} V^H b \). All of the coefficient matrices are the same, while only \( z \) varies in \( Z_2 \). Thus, we are able to use \texttt{hess}(\( W^H EV, W^H AV \)) and \texttt{linsolve}(\ldots, \texttt{opt.UHESS}=1) for reducing CPU times.

It is a problem how to choose \( t_{l+1} \) for the left subspace, since we need two new shifts for adding one order. We make an easy choice by \( t_{l+1} = \overline{s_{l+1}} \). There are other options, such as

\[
\begin{align*}
\text{Option 2 : } & \quad t_{l+1} = \arg \max_{z \in Z_2} \frac{\varphi_l(z) \psi_l(z)(z - s_{l+1})}{|\Lambda(z)|^2}, \\
\text{Option 3 : } & \quad t_{l+1} = \arg \max_{z \in Z_2} \frac{\varphi_l(z) \psi_l(z)(z - s_{l+1})}{|\Lambda(z)|^2} \| (zW^H EV - W^H AV)^{-1} W^H b \|_2, \\
\text{Option 4 : } & \quad t_{l+1} = \arg \max_{z \in Z_2} \frac{\varphi_l(z) \psi_l(z)(z - s_{l+1})}{|\Lambda(z)|^2} |c^H V(zW^H EV - W^H AV)^{-1} W^H b|.
\end{align*}
\]

Numerical testing do not show these options have better behaviors than \( t_{l+1} = \overline{s_{l+1}} \).
We measure the $H_\infty$ norm error by the max error:

$$\|e(z)\|_\infty = \max_{z \in Z_e} |h(z) - \tilde{h}(z)|,$$

(5.5)

where $Z_e$ also has form (5.4). Our greedy algorithms actually do not need to compute it. It is only used for the evaluations with other algorithms. To compute the max error, we shall spend much computation. It is not like the case of matrix equations, whose residual norm can be computed in the reduced problems [47, 48].

6. Numerical experiments. All experiments are carried out in Matlab2016a on a notebook (64 bits) with an Intel CPU i7-5500U and 8GB memory. Any data involving random numbers are fixed by setting randn('state',0) or rand('state',0). Note eigs uses a random vector as the initial vector. Before we use eigs for computing (5.2), we also set rand('state',0). We compare our algorithms with ARKSM (Algorithm 1), AAA and IRKA.

Algorithm AAA can be applied for MOR [2, 20, 53]. It solves a min-max problem. Thus, it approximately solves the $H_\infty$ norm MOR problem. The algorithm gets samples on the image axis [53, Section 6.9]. The greedy idea is also used, and thus the selected samples are nested. In our testing, the optional samples set $Z_A$ has the same form of $Z(\alpha, \beta, k)$. If $Z_A = Z_e$, then AAA outputs the error directly. This is actually an attractive advantage of AAA.

$H_2$ norm MOR is accomplished by IRKA [8, 34]. It mainly has two disadvantages: it converges slowly and the optimal shifts are not nested. The advantage is that it has optimization property in $H_2$ norm sense. IRKA actually does not need to compute the model error either in $H_2$ or $H_\infty$ norm, since it is automatically optimized in $H_2$ norm sense. Here, we still compute its max error (5.5) to be a rough standard for other algorithms. The initial shifts of IRKA are the outputs shifts of ARKSM. We stop IRKA if the iteration number is larger than $100$ or $\|S_j - S_{j-1}\|_2 < 10^{-6}\|S_j\|_2$, where $S_j$ is the sorted shifts vector at $j$th iteration.

In all testings, we use Matlab backslash to do the inversion $(A - s_iE)^{-1}b$. In Matlab, directly using backslash to finish $(A - s_iE)^{-H}c$ is usually faster than saving LU decomposition factors of $(A - s_iE)$ and solving triangle linear equations. Thus, we use the former in IRKA.

For large scale problems, the computation of all of the algorithms concentrates on the linear solvers. To get $l$ order MOR, we account the number of linear solvers for every algorithm. AAA needs to “get samples” on the imaginary axis. It computes $h(z)$ for $z \in Z_A = Z(\alpha, \beta, k_A)$. Thus, it needs $(2k_A + 1)$ linear solvers. IRKA needs $2j_{\max}l$ linear solvers, where $j_{\max}$ is the final iteration number when IRKA stops. ARKSM needs $l$ linear solvers, while our two-sided algorithm needs $2l$ linear solvers. Note ARKSM is an one-sided type algorithm.

Example 1 (small problems): The testing examples are from SLICOT benchmark problems [15]. We set $b = B(:,1)$ and $c = C(1,:)'$, if the model problems have multi inputs and multi outputs. We set $Z_A = Z_e = Z(-3,5,700)$ for computing the max error and the samples set for AAA. We use $Z_2 = Z(-3,5,500)$ as the optional samples for selecting shifts in two-sided algorithms.

The error pictures of two problems are showed in Fig. 6.1. The CPU times of 40 order MOR are listed in Table 6.1. Except $H_2$ norm MOR (IRKA), other algorithms have nested shifts. Thus, in Table 6.1, we only compute the $H_2$ norm MOR for $l = 40$. Other codes for making Fig. 6.1 and Table 6.1 do not have big differences.

Example 2 (large scale problems): L10000 and L10648 are from papers [19] and [63] respectively, with $E = I$. They are acquired from the explicit discretization of partial differential equations. The left are from Oberwolfach collection [42]. The other information are summarized in the first part of Table 6.2.

We set $Z_A = Z_e = Z(\alpha, \beta, 400)$ and $Z_2 = Z(\alpha, \beta, 500)$. The error pictures of two problems are showed in Fig. 6.2, and CPU times of 40 order MOR are listed in Table 6.2. Other settings are the same as the one for small problems.

We give some observation here:

1. In Tables 6.1 and 6.2, the CPU times of AAA include the one of “get samples”. Note that other algorithms actually do not need to “get samples”. We still “get samples” for computing the max error (5.5), so that all of the algorithms can be compared in the same sense.
Table 6.1: 40 order MOR of small problems

|         | Matrix | BEAM | CDPLAYER | EADY | FOM | ISS | RANDOM |
|---------|--------|------|----------|------|-----|-----|--------|
| CPU(s)  | Get Samples | 7.08 | 0.20 | 40.13 | 0.51 | 0.40 | 3.76 |
|         | AAA    | 7.67 | 0.72 | 40.66 | 0.80 | 1.01 | 4.11 |
|         | ARKSM  | 2.96 | 2.62 | 3.87  | 2.67 | 2.64 | 2.91 |
|         | two-sided(O1) | 3.21 | 2.72 | 5.61  | 2.92 | 2.84 | 3.04 |
|         | two-sided(O2) | 5.02 | 4.72 | 7.03  | 4.61 | 4.60 | 4.79 |
|         | $H_2$(IRKA) | 44.85 | 0.78 | 235.87 | 4.18 | 2.02 | 23.60 |

∥$e(z)$∥∞

|         | AAA    | 5.83E−02 | 2.29E−03 | 2.28E−06 | 5.96E−12 | 4.54E−06 | 1.21E−09 |
|         | ARKSM  | 1.29E+01 | 3.87E+01 | 9.88E−04 | 5.01E−12 | 4.05E−03 | 1.61E−06 |
|         | two-sided(O1) | 1.12E+00 | 1.02E−01 | 1.58E−05 | 1.02E−11 | 4.26E−05 | 6.67E−09 |
|         | two-sided(O2) | 6.76E−01 | 9.25E−02 | 7.51E−06 | 3.72E−12 | 2.68E−05 | 5.25E−09 |
|         | $H_2$(IRKA) | 4.24E−02 | 2.49E−02 | 9.77E−07 | 4.32E−12 | 1.57E−05 | 3.18E−09 |

IRKA#iter

| AAA | H2(IRKA) | ARKSM | two-sided(O2) |
|-----|---------|-------|---------------|
| 100 | 39      | 100   | 100           |
| 100 | 100     | 62    | 100           |

“Get Samples” accounts the CPU times of computing $h(z)$ for $z \in Z_3 = Z_e = Z(-3, 5, 700)$. As is stated in Fig. 6.1, the data of AAA only involves $l = 29$ for FOM and $l = 31$ for RANDOM. Here, we do not compute $H_2$ norm MOR (IRKA) for $l < 40$. The initial shifts of IRKA are from the output shifts of Algorithm ARKSM. “IRKA#iter” denotes the iteration number of IRKA when it stops.

Fig. 6.1: Behaviors of different MOR for small problems

![Graph](image1.png)

Although we input $l = 40$ into AAA, it stops at $l = 31$ for RANDOM.

2. In Fig. 6.2, the error pictures of the two-sided(O2) algorithm are close to the one of $H_2$ norm MOR and AAA. Since $H_2$ norm MOR has $H_2$ norm optimality and AAA’s nice effectiveness is already tested in many examples [53], we can say our algorithms for solving problem (4.3) behavior well. Meanwhile, our two-sided(O2) algorithm spends much less time than IRKA and AAA in large scale problems.

3. Both $H_2$ norm MOR and our two-sided algorithm are two-sided type projection method. For 40 order,
they actually have 80 shifts. ARKSM is actually an one-sided type projection method. For 40 order, it only has 40 shifts. In Section 3, we find the errors of $l$ order two-sided and $2l$ order one-sided methods are quite similar. Thus, we think 20 order two-sided algorithm will have the similar precision like 40 order onesided algorithm. Some of error pictures in Fig. 6.1 and 6.2 roughly show this fact, e.g., EADY, RANDOM and rail20209. Concretely speaking, the max error of $l = 40$ in ARKSM approximately equals to the one of $l = 20$ in two-sided algorithm or $H_2(\text{IRKA})$.

7. Conclusion. We have the following contributions: 1. We obtain the explicit formula for the model error by rational Krylov subspaces. It is a conclusive result of moments matching results. Our result about the error is intrinsic. From the three explanations, we know the error is a Gauss quadrature remainder or Hermitian formula remainders. Whether a quadrature formula has the remainder formula or not is important to the method. Whether an interpolation formula has the remainder formula or not is important to the method. Our explicit error formula is helpful for the researchers to analyze the MOR error when various rational Krylov subspaces are used. 2. We find the error is the interpolation remainder of Gauss quadrature, when the Gauss quadrature is applied on the resolvent function $H(\lambda, z) = 1/(z - \lambda)$. This also explains why an $l$ order two-sided projection method have the similar expression like a $2l$ order one-sided projection method. The $l$ order two-sided projection method has $(2l - 1)$ precision, so does the one-sided projection method. 3. We discover the error is also the remainder when Hermitian formula is applied on the resolvent function with respect to variables $z$ and $\lambda$. 4. We transform the interpolatory $H_\infty$ norm MOR into the approximation of matrix function. Thus, the logarithmic potential theory can been used. Since the error of the rational interpolation for the resolvent function can been expressed explicitly, the approach to solving interpolatory $H_\infty$ norm MOR should been reconsidered. 5. By using the error formula, we propose a greedy two-sided projection method for interpolatory $H_\infty$ norm MOR.

We would like to mention another two points, whose phenomena are known. 1. The error formula is independent of the stability of $A$. Thus, the two-sided projection method can not maintain the stability of the system. 2. The final error formula is independent of the bases. For numerical stabiility, the researchers prefer to the orthonormal bases in both left and right subspaces.

It is a problem how to generalize the error formula to the multi-input-multi-output system. Once the concise and explicit expressions of the residuals can been obtained, then the error formula of the full interpolation
Section 3.3] can be obtained by \( e(z) = R^H_0(zI - A)^{-1}R_B \). [25, Theorem 2.9] describes some properties of the residuals, but a more concise expression is still appreciated. Another attempt is to use the tangential interpolation. When the left and right tangential directions do not compute \( H \), \( \{i\} \) \( \{b_i\} \) \( \{c_i\} \) are stated in [3, Section 5.3]. By (5.2), \( 10^m \) is selected as a lower bound of \( \|s_{\max}\| \), so \( 10^3 \) an upper bound of \( \|s_{\min}\| \). “Get Samples” accounts the CPU times of evaluating \( h(z) \) for \( z \in \mathbb{C} \). Here, we do not compute \( H_2 \) norm MOR (IRKA) for \( l < 40 \). The initial shifts of IRKA are from the output shifts of Algorithm ARKSM. “IRKA\#\#iter” denotes the iteration number of IRKA when it stops.

**Acknowledgment.** The author deeply appreciates Valeria Simoncini, Ren-cang Li and Shengxin Zhu for their insightful comments.

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