AN ERROR ANALYSIS FOR RATIONAL GALERKIN PROJECTION APPLIED TO THE SYLVESTER EQUATION*

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Abstract. In this paper we suggest a new formula for the residual of Galerkin projection onto rational Krylov spaces applied to a Sylvester equation, and establish a relation to three different underlying extremal problems for rational functions.

These extremal problems enable us to compare the size of the residual for the above method with that obtained by ADI. In addition, we deduce several new a priori error estimates for Galerkin projection onto rational Krylov spaces, both for the Sylvester and for the Lyapunov equation.

Key words. Sylvester equation, Lyapunov equation, Galerkin projection, rational Krylov spaces, ADI

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1. Introduction.

Given two square matrices $A \in \mathbb{C}^{M\times M}, B \in \mathbb{C}^{N\times N}$, not necessarily of the same size, with disjoint spectra $\Lambda(A)$, $\Lambda(B)$, the Sylvester equation

$$\mathcal{S}_{A,B}X := AX - XB = C \tag{1.1}$$

has a unique solution $X = \mathcal{S}_{A,B}^{-1}C \in \mathbb{C}^{M\times N}$ for all $C \in \mathbb{C}^{M\times N}$. One obtains for the special case $B = -A^*$ and $C = C^*$ the so-called Lyapunov equation. Here the star denotes complex conjugation and transposition.

Sylvester equations appear frequently in many areas of applied mathematics, see for instance the survey [10] and the references therein. For instance, Sylvester equations occur naturally in matrix eigendecompositions [22], control theory [14], model reduction [1, 2, 33], but also numerical solutions of Riccati equations [18], or image processing [12]. In many of these applications, A, B are fairly large and sparse, and C is of low rank $d \ll M, N$, so that direct methods for solving (1.1) are not suitable. In this case we will use a full rank factorization of the right-hand side

$$C = ab^*, \qquad a \in \mathbb{C}^{M\times d}, \quad b \in \mathbb{C}^{N\times d}.$$

In order to simplify presentation, we will deal in this paper with the case $d = 1$, the statements for the case $d > 1$ are similar, but since some tangential interpolation problems are involved we leave this for another paper.

The aim of this paper is to compare error estimates for two popular iterative methods for solving (1.1). The ADI iteration due to Peaceman and Rachford [27] has been adapted by Wachspress [35, 36] for solving (1.1), see also related work by Birkhoff and Varga [11]. Roughly speaking, this method requires parameters $z_{A,1}, ..., z_{A,n} \in \mathbb{C} \setminus \Lambda(A)$ and $z_{B,1}, ..., z_{B,n} \in \mathbb{C} \setminus \Lambda(B)$ and computes an approximation X_n^{ADI} of rank nd by solving shifted systems with coefficient matrices $(z_{A,j}I - A)$ and $(z_{B,j}I - B)$. Two aspects make the ADI method particularly attractive. First, it is possible to implement the method through full rank decompositions of the iterates X_n^{ADI}, and thus it essentially remains to solve $2n$ shifted systems with d right-hand sides, see [9] and the references therein. Another attractive aspect is that the ADI error $X - X_n^{ADI}$

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and the ADI residual $\mathcal{S}_{A,B}(X - X_n^{ADI})$ can be described via very simple formulas, namely

$$X - X_n^{ADI} = R^{ADI}(A)^{-1} X R^{ADI}(B), \tag{1.2}$$

$$\mathcal{S}_{A,B}(X - X_n^{ADI}) = R^{ADI}(A)^{-1} ab^* R^{ADI}(B), \tag{1.3}$$

with the rational function

$$R^{ADI}(z) = \prod_{j=1}^{n} \frac{z - z_{A,j}}{z - z_{B,j}}.$$

It turns out that with a "nearly" optimal choice of parameters the ADI error is small even for modest values of n, but this is no longer true if the parameters are not well chosen, and here it makes sense to consider instead projection methods.

Given matrices with orthonormal columns

$$U \in C^{M\times m}, \quad U^*U = I, \qquad V \in C^{N\times n}, \quad V^*V = I, \tag{1.4}$$

for the Galerkin approach one looks for an approximant of the form $X_{m,n}^G = UY^GV^*$ with $Y^G \in \mathbb{C}^{m\times n}$ by requiring that the residual satisfies the orthogonality conditions

$$U^* \mathcal{S}_{A,B}(X - X_{m,n}^G) V = 0.$$

Introduce the projected Rayleigh matrices

$$A_m := U^*AU \in \mathbb{C}^{m\times m}, \quad B_n := V^*BV \in \mathbb{C}^{n\times n}, \tag{1.5}$$

and suppose that $\Lambda(A_m) \cap \Lambda(B_n)$ is empty. Then it is not difficult to check the following formula for the Galerkin approximant

$$X_{m,n}^G = UY^GV^*, \quad Y^G = \mathcal{S}_{A_m,B_n}^{-1}(a_m b_n^*), \tag{1.6}$$

where

$$a_m := U^*a, \quad b_n := V^*b. \tag{1.7}$$

Here we suppose that $m, n \ll M, N$, making it possible to solve the Sylvester equation $S_{A_m,B_n}Y = A_mY - YB_n = a_m b_n^*$ by, e.g., some direct method, and to compute the above quantities A_m, U, a_m, B_n, V, b_n in reasonable time. One big advantage of such projection methods is that for the fields of values we have the inclusions $W(A_m) \subset W(A)$, and $W(B_n) \subset W(B)$.

For parameters $z_{A,1}, ..., z_{A,m} \in \overline{\mathbb{C}} \setminus \Lambda(A)$ and $z_{B,1}, ..., z_{B,n} \in \overline{\mathbb{C}} \setminus \Lambda(B)$, $\overline{\mathbb{C}}$ denoting the extended complex plane $\mathbb{C} \cup \{\infty\}$, we introduce the polynomials

$$Q_A(z) = \prod_{j=1, z_{A,j}\neq\infty}^{m} (z - z_{A,j}), \quad Q_B(z) = \prod_{j=1, z_{B,j}\neq\infty}^{n} (z - z_{B,j}), \tag{1.8}$$

and denote by $\mathcal{P}_k$ the space of polynomials with complex coefficients of degree at most k. The rational Krylov spaces

$$\begin{aligned} \mathcal{K}_{A,m} &= \{R_A(A)a : R_A \in \mathcal{P}_{m-1}/Q_A\}, \\ \mathcal{K}_{B^*,n} &= \{R_B(B)^*b : R_B \in \mathcal{P}_{n-1}/Q_B\}, \end{aligned} \tag{1.9}$$

built with help of rational functions of fixed denominator play a particular role in the construction of the ADI method, indeed in the case $m = n$ we find that

$$\mathrm{colspan}(X_n^{ADI}) \subset \mathcal{K}_{A,n}, \qquad \mathrm{colspan}((X_n^{ADI})^*) \subset \mathcal{K}_{B^*,n},$$

where up to some degenerate cases there holds equality in both inclusions. Hence in what follows we will always suppose that the columns of U, and of V, form an orthonormal basis of $\mathcal{K}_{A,m}$, and of $\mathcal{K}_{B^*,n}$, respectively, which makes sense to compare the errors for ADI and for Galerkin projection onto rational Krylov spaces (or shorter rational Galerkin).

The original idea of projecting onto polynomial Krylov spaces (all parameters $z_{A,j}, z_{B,j} = \infty$) probably goes back to Saad [29], the case of rational Krylov spaces has been considered subsequently by many authors, see for instance [19, 20, 21] and the references therein. However, to our knowledge, until recently little was known about a priori error estimates in the spirit of the famous CG estimate in terms of the condition number. We found first results in this direction by Penzl [28], followed by Druskin and Simoncini [32] and by Kressner and Tobler [25]. The work of [32, 25] is based on an integral representation for the solution X of the Sylvester equation (1.1) in terms of the exponential function. There exists another integral representation in terms of resolvents

$$X = \frac{1}{2\pi i} \int_\Gamma (zI - A)^{-1} ab^* (zI - B)^{-1} \, dz, \tag{1.10}$$

the curve Γ encircling once the eigenvalues of A but not those of B. This integral formula has been the starting point for similar a priori error estimates for so-called extended Krylov spaces (all parameters $z_{A,j}, z_{B,j} \in \{0, \infty\}$) in [24], see also [25]. The case of arbitrary rational Krylov spaces was considered by Druskin, Knizhnerman and Simoncini in [16] using elegant but deep tools from complex approximation theory like Takenaka-Malmquist orthogonal rational functions and Faber-Dzhrbashyan rational functions; we will summarize all these findings in §2.4 below. The results in [16] are more general but weaker than those of [32, 25, 24] in the sense that the authors only obtain nth root asymptotic upper bounds for the error, with an explicit convergence factor given in terms of the parameters $z_{A,j}$ and the fields of values of the matrices A and B.

Tools from approximation theory also have been an important argument in [25, Theorem 4.3 and Eqn. (39)] where the authors suggest for the Lyapunov equation with selfadjoint positive definite $A = -B^*$ to consider a bivariate polynomial approximation problem.

Our approach is based on an orthogonal decomposition of the residual for rational Galerkin in Theorem 2.1 below, which to our knowledge is new, and which conceptually differs from the one given for instance in [17, Proposition 4.1], the latter being an immediate consequence of the representation of $AU - UA_m$ for rational Krylov projections. Each of the three terms in our new representation of the residual can be related to some extremal problem for (univariate) rational functions with prescribed poles. The starting point for this new residual formula is the observation that enforcing the residual to be orthogonal reminds of the well-known FOM method for solving systems of linear equations. Thus we may use in (1.10) a well-known formula for the FOM error for shifted systems, given, e.g., in [5].

As a consequence, we are able to relate in Corollary 2.2 the residual norms of both ADI and the rational Galerkin method. We obtain in Theorem 2.3 an explicit a priori estimate for the rational Galerkin residual for couples A, B having disjoint field of values, and state an improved formula for A, B being selfadjoint. The particular case of a Lyapunov equation is studied in Corollary 2.5, which enables us to compare in §2.4 the upper bounds proposed in this paper to existing work. In particular, our upper bounds describe a geometric convergence behavior, with the same convergence factor as that discussed in [16].

The rest of the paper is organized as follows. Section 2 contains further definitions and the statements of our main results, together with motivating remarks. The proofs for these statements can be found in Section 3. In particular, good candidates for our rational and matrix-valued extremal problems are constructed in Theorem 3.4, generalizing previous work [4] for polynomial matrix–valued extremal problems like matrix Chebyshev polynomials.

Notation. In what follows, $\|\cdot\|$ denotes the Euclidian vector norm and the spectral matrix norm, whereas by $\|\cdot\|_F$ we denote the Frobenius norm. The field of values of a square matrix A is defined by $W(A) = \{y^* A y : \|y\| = 1\}$, which is known to be always convex and compact. By stacking the columns of X, C in a large column vector, one may rewrite (1.1) as an ordinary system of equations $\mathcal{M}x = c$ with $\mathcal{M} = I_N \otimes A - B^T \otimes I_M$. It is not difficult to show that $W(\mathcal{M}) = W(A) - W(B)$, see for instance [16, Proof of Theorem 4.2]. As a consequence, in the case $W(A) \cap W(B)$ being empty, we may give simple estimates for the norm of our Sylvester operator and its inverse

$$\|\mathcal{S}_{A,B}\| = \sup_C \frac{\|\mathcal{S}_{A,B}C\|_F}{\|C\|_F} = \|\mathcal{M}\| \leq 2\,\mathrm{diam}(W(A), W(B)), \tag{1.11}$$

$$\|\mathcal{S}_{A,B}^{-1}\| = \sup_C \frac{\|C\|_F}{\|\mathcal{S}_{A,B}C\|_F} = \|\mathcal{M}^{-1}\| \leq \frac{1}{\mathrm{dist}(W(A), W(B))} \tag{1.12}$$

$$\text{where} \quad \mathrm{diam}(W(A), W(B)) := \max_{\substack{x \in W(A) \\ y \in W(B)}} |x - y|. \tag{1.13}$$

2. Statement of results.

2.1. A new formula for the residual for rational Galerkin. In order to state our main results, we need to introduce some particular rational functions

$$R_A^G(z) = \frac{\det(zI - A_m)}{Q_A(z)} \in \mathcal{P}_m/Q_A, \quad R_B^G(z) = \frac{\det(zI - B_n)}{Q_B(z)} \in \mathcal{P}_n/Q_B, \tag{2.1}$$

where Q_A, Q_B are as in (1.8). From the theory of rational Krylov spaces it is known that

$$U^* R_A^G(A) a = 0, \quad V^* R_B^G(B)^* b = 0, \tag{2.2}$$

in other words, $R_A^G(A)a \in \mathcal{K}_{A,m+1}$ together with the columns of U form an orthogonal basis of $\mathcal{K}_{A,m+1}$, and, similarly $R_B^G(B)^* b \in \mathcal{K}_{B^*,n+1}$ together with the columns of V form an orthogonal basis[1] of $\mathcal{K}_{B^*,n+1}$.

Notice that, by construction, the residual $\rho = \mathcal{S}_{A,B}(X - X_{m,n}^G)$ has columns in $\mathcal{K}_{A,m+1}$, and its adjoint has columns in $\mathcal{K}_{B^*,n+1}$. The following result tells us how to represent the residual in these orthogonal bases.

[1]We keep the same denominators in the rational Krylov spaces, or, equivalently, we take the new poles $z_{A,m+1} = z_{B,n+1} = \infty$.

THEOREM 2.1. *Let $d = 1$, and write shorter $\rho = \mathcal{S}_{A,B}(X - X^G_{m,n})$ for the rational Galerkin residual. Then $\rho = \rho_{1,2} + \rho_{2,1} + \rho_{2,2}$, with*

$$\rho_{1,2} = U \frac{1}{R^G_B}(A_m) a_m b^* R^G_B(B), \quad \rho_{2,1} = R^G_A(A) a b^*_n \frac{1}{R^G_A}(B_n) V^*, \tag{2.3}$$
$$\rho_{2,2} = \frac{R^G_A(A) a b^* R^G_B(B)}{R^G_A(\infty) R^G_B(\infty)},$$

and in particular

$$\|\rho\|^2_F = \|\rho_{1,2}\|^2_F + \|\rho_{2,1}\|^2_F + \|\rho_{2,2}\|^2_F. \tag{2.4}$$

If $W(A) \cap W(B)$ is empty, each term is the minimal value of some extremal problem

$$\|\rho_{2,2}\|_F = \inf_{\substack{R_A \in \frac{\mathcal{P}_m}{Q_A} \\ R_B \in \frac{\mathcal{P}_n}{Q_B}}} \left\| \frac{R_A(A) a b^* R_B(B)}{R_A(\infty) R_B(\infty)} \right\|_F = \|(I - UU^*) a b^* (I - VV^*)\|_F, \tag{2.5}$$

$$\|\rho_{1,2}\|_F = \min_{R_B \in \frac{\mathcal{P}_n}{Q_B}} \left[\left\| \frac{1}{R_B}(A_m) a_m b^* R_B(B) \right\|_F + c_0 \left\| \frac{1}{R_B}(A_m) a_m b^*_n R_B(B_n) \right\|_F \right], \tag{2.6}$$

$$\|\rho_{2,1}\|_F = \min_{R_A \in \frac{\mathcal{P}_m}{Q_A}} \left[\left\| R_A(A) a b^*_n \frac{1}{R_A}(B_n) \right\|_F + c_0 \left\| R_A(A_m) a_m b^*_n \frac{1}{R_A}(B_n) \right\|_F \right], \tag{2.7}$$

where $c_0 := 2\, diam(W(A), W(B))/dist(W(A), W(B))$. For each extremal problem (2.5), (2.6), and (2.7), the minimum is attained for $R_A = R^G_A$ and $R_B = R^G_B$.

From (2.5) we see that $\rho_{2,2} = 0$ provided that one of the poles $z_{A,j}$ or $z_{B,j}$ is chosen to be ∞ (as for instance in [24, 25, 32] where $z_{A,1} = z_{B,1} = \infty$), since then either $a \in \mathcal{K}_{A,m}$ or $b \in \mathcal{K}_{B^*,n}$.

2.2. Rational Galerkin versus ADI. By comparing the expression (1.3) with Theorem 2.1 it is not difficult to see that $X^{ADI}_n = X^G_{n,n}$ provided that the poles $z_{A,j}$, and $z_{B,j}$, coincide with the nth Ritz values of B and A, respectively (i.e., the eigenvalues of B_n and A_n), since then $R^{ADI} = R^G_B = 1/R^G_A$. This observation was already mentioned, e.g., in [16, Theorem 3.4]. However, it is quite difficult to choose such poles since of course the Ritz values depend on the poles.

Theorem 2.1 allows us to compare the size of the residual for the ADI method with that of rational Galerkin for arbitrary poles. A weaker result in this direction can be found in [16, Theorem 4.2] where the authors show that the rational Galerkin error is always smaller than a (classical) upper bound for the ADI error.

COROLLARY 2.2. *Provided that $W(A) \cap W(B)$ is empty, we have for the residuals*

$$\|\mathcal{S}_{A,B}(X - X^G_{n,n})\|_F \le C\, \|\mathcal{S}_{A,B}(X - X^{ADI}_n)\|_F,$$

with a constant $C \le 3 + 2c_0$ with c_0 from Theorem 2.1 independent of the parameters $z_{A,j}, z_{B,j}$.

We do not claim of having found the optimal value of the constant C. However, it becomes clear from Corollary 2.2 that, even for optimal poles, ADI cannot give much better results as rational Galerkin. Recall that for poor poles ADI is known to give much larger residuals [9].

2.3. Explicit bounds for the residual of rational Galerkin. We now state some a priori upper bounds for the residual of the rational Galerkin method in terms of the fields of values of A and B. In case of selfadjoint A, recall that $W(A) = [\lambda_{\min}(A), \lambda_{\max}(A)]$, and that $\|f(A)\| \leq \|f\|_{L^\infty(W(A))}$ for any function f analytic on $W(A)$. Crouzeix [13] showed recently the deep result that there exists a universal constant $C_{Crouzeix} \leq 11.08$ (he conjectures that $C_{Crouzeix} = 2$) such that $\|f(A)\| \leq C_{Crouzeix} \|f\|_{L^\infty(W(A))}$ for any matrix A and any function f analytic on $W(A)$. This makes the field of values quite attractive for matrix function analysis, though in general field–of–value estimates may be pessimistic.

Theorem 2.1 tells us that for upper bounds of the rational Galerkin residual it is useful to have upper bounds for the matrix-valued rational extremal problem

$$E_m(A, Q_A, z) := \min_{P \in \mathcal{P}_m} \frac{\|\frac{P}{Q_A}(A)\|}{|\frac{P}{Q_A}(z)|}, \quad z \in \overline{\mathbb{C}}, \tag{2.8}$$

which for $z = \infty$ and $z_{A,j} \to \infty$ is related to a matrix Chebyshev extremal problem studied by several authors, see, e.g., [34] and the references therein. Indeed, according to (2.5), for $\rho_{2,2}$ we require $E_m(A, Q_A, \infty)$ and $E_n(B, Q_B, \infty)$, whereas, according to (2.7), for bounding $\rho_{2,1}$ (and similarly $\rho_{1,2}$) we can use the upper bound

$$\min_{P \in \mathcal{P}_m} \|\frac{P}{Q_A}(A)\| \, \|\frac{Q_A}{P}(B)\| \leq C_{Crouzeix} \max_{z \in W(B)} E_m(A, Q_A, z).$$

Notice that such kind of estimates are potentially not very sharp, though (up to the factor $C_{Crouzeix}$) there exist sequences of normal matrices for which asymptotically equality is attained. Again using the Crouzeix estimate we may relate (2.8) with the quantity

$$E_m(\mathbb{E}, Q_A, z) := \min_{P \in \mathcal{P}_m} \frac{\|\frac{P}{Q_A}\|_{L^\infty(\mathbb{E})}}{|\frac{P}{Q_A}(z)|}, \quad z \in \overline{\mathbb{C}}, \quad \mathbb{E} \subset \mathbb{C}, \tag{2.9}$$

here for $\mathbb{E} = W(A)$. As we will see in Theorem 3.4 below, it is possible for convex $\mathbb{E}$ and in particular for $\mathbb{E} = W(A)$ to give an explicit upper bound both for $E_m(A, Q_A, z)$ and for $E_m(\mathbb{E}, Q_A, z)$ which (knowing only $W(A)$) can be at most improved by a modest factor. Notice that lower bounds for $E_m(\mathbb{E}, Q_A, z)$ and arbitrary $\mathbb{E}$ are easily obtained by the rational version of the Bernstein-Walsh inequality due to Gonchar [23], see also [16, Lemma 4.4], and Theorem 3.4 below.

In order to describe the rate of convergence, we denote by $g_A(\cdot, \zeta)$ the Green function of $\overline{\mathbb{C}} \setminus W(A)$ with pole at $\zeta \in \overline{\mathbb{C}}$, see [31], and define

$$u_{A,m}(z) = \exp\Big(-\sum_{j=1}^{m} g_A(z, z_{A,j})\Big).$$

Recall from [31, §I.1.4] that Green functions satisfy $g_A(z, \zeta) > 0$ for $z, \zeta \notin W(A)$, and $g_A(z, \zeta) = 0$ else. If we disregard the particular case $z_{A,1}, ..., z_{A,m} \in W(A)$, we may conclude that $0 \leq u_{A,m}(z) < 1$ for all $z \notin W(A)$ including $z = \infty$, and that $u_{A,m}(z_{A,j}) = 0$ if $z_{A,j} \notin W(A)$.

Similarly, we define

$$u_{B,n}(z) = \exp\Big(-\sum_{j=1}^{n} g_B(z, z_{B,j})\Big).$$

We remark that in case of selfadjoint matrices we may make the expressions for $u_{A,m}$, and $u_{B,n}$, more explicit: the Green function g for a real interval $[\alpha,\beta]$ is known to be

$$g(z,\zeta) = \log \Big| \frac{\sqrt{\frac{z-\beta}{z-\alpha}}\sqrt{\frac{\overline{\zeta}-\alpha}{\overline{\zeta}-\beta}}+1}{\sqrt{\frac{z-\beta}{z-\alpha}}\sqrt{\frac{\zeta-\alpha}{\zeta-\beta}}-1} \Big|$$

with the principal branch of the square root, $\sqrt{1}=1$, and thus

$$u_{A,m}(z) = \prod_{j=1}^{m} \Big| \frac{\sqrt{\frac{z-\lambda_{\max}(A)}{z-\lambda_{\min}(A)}}\sqrt{\frac{z_{A,j}-\lambda_{\min}(A)}{z_{A,j}-\lambda_{\max}(A)}}-1}{\sqrt{\frac{z-\lambda_{\max}(A)}{z-\lambda_{\min}(A)}}\sqrt{\frac{\overline{z_{A,j}}-\lambda_{\min}(A)}{\overline{z_{A,j}}-\lambda_{\max}(A)}}+1} \Big|. \tag{2.10}$$

We have the following result.

THEOREM 2.3. *Let $d=1$ and $W(A)\cap W(B)$ be empty, and define*[2]

$$\gamma_{A,B} := \max_{z\in W(B)} u_{A,m}(z), \qquad \gamma_{B,A} := \max_{z\in W(A)} u_{B,n}(z),$$

then we have for the rational Galerkin residual and for general A,B,

$$\frac{\|S_{A,B}(X-X^G_{m,n})\|_F}{\|a\|\,\|b\|} \le 4c_1 \max\{\gamma_{A,B},\gamma_{B,A}\} + c_2\Big(\frac{2\gamma_{A,B}}{1-\gamma_{A,B}} + \frac{2\gamma_{B,A}}{1-\gamma_{B,A}}\Big),$$

where

$$c_1 = \min_{\substack{j=1,\ldots,m\\ k=1,\ldots,n}} \frac{1}{(1-\exp(-g_A(z_{A,j},\infty)))(1-\exp(-g_B(z_{B,k},\infty)))}$$

measuring how far the "furthest" pole is from the fields of values, and $c_2 = (1+c_0)\,C_{Crouzeix}$ with c_0 from Theorem 2.1. For selfadjoint A,B and $\{z_{A,1},...,z_{A,m}\}$, $\{z_{B,1},...,z_{B,n}\}$ closed under complex conjugation, we have the improvement

$$\frac{\|S_{A,B}(X-X^G_{m,n})\|_F}{\|a\|\,\|b\|} \le 4\max\{\gamma_{A,B},\gamma_{B,A}\} + c_3(\gamma_{A,B}+\gamma_{B,A})$$

with

$$c_3 = 2\sqrt{2\frac{\max\{|\lambda_{\min}(B)-\lambda_{\max}(A)|,|\lambda_{\min}(A)-\lambda_{\max}(B)|\}}{\min\{|\lambda_{\min}(B)-\lambda_{\max}(A)|,|\lambda_{\min}(A)-\lambda_{\max}(B)|\}}}.$$

REMARK 2.4. *We learn from the upper bounds of Theorem 2.3 that we should keep both $\gamma_{A,B}$* **and** *$\gamma_{B,A}$ small. Optimizing $\gamma_{A,B}$ can be done by choosing $z_{A,j}$, and optimizing $\gamma_{B,A}$ can be done by choosing $z_{B,j}$. We claim here without proof (being a consequence of [31, Theorem VIII.2.3]) that*

$$\gamma_{A,B}^{1/m} \ge R(W(A),W(B))^{-1}, \quad \gamma_{B,A}^{1/n} \ge R(W(A),W(B))^{-1},$$

[2] For simplifying notation we do not display the dependency on m,n which in what follows are always supposed to be fixed. However, all appearing explicit constants c_0,c_1,c_2 do not depend on m and n.

with $R(W(A), W(B))$ the Riemann modulus of the doubly connected domain $\overline{\mathbb{C}} \setminus (W(A) \cup W(B))$, and that both inequalities are asymptotically sharp, since they can be attained by appropriate choices of the poles. $\square$

It is worthy to write down the bounds of Theorem 2.3 for the special case $B = -A^*$ of a Lyapunov equation and $m = n$. We will make some simplifying assumptions.

COROLLARY 2.5. *Consider a Lyapunov equation ($B = -A^*$) with $d = 1$ and $m = n$ and $W(A) \cap (-W(A))$ being empty. We suppose in addition that A has real entries, and that the poles are chosen such that $z_{A,j} = -z_{B,j}$ occur in conjugate pairs. Then with c_0, c_2 as before*

$$\frac{\|S_{A,B}(X - X^G_{n,n})\|_F}{\|a\| \, \|b\|} \leq (4 + 4c_2) \frac{\gamma_{A,B}}{(1 - \sqrt{\gamma_{A,B}})^2}.$$

If in addition A is selfadjoint (and hence positive or negative definite) then we have the improvement

$$\frac{\|S_{A,B}(X - X^G_{n,n})\|_F}{\|a\| \, \|b\|} \leq (4 + 4\sqrt{2 \, cond(A)}) \, \gamma_{A,B}.$$

Proof. Since A has real entries, we get that $W(A)$ is symmetric with respect to the real axis, and thus $W(B) = W(-A^*) = -W(A)$. Also, by our symmetry assumptions on the poles,

$$u_{A,n}(z) = u_{A,n}(\overline{z}) = u_{B,n}(-z), \quad \gamma_{A,B} = \gamma_{B,A}.$$

Therefore, as in the proof of the first part of Theorem 2.3 we conclude that $u_{A,n}(\infty) = u_{B,n}(\infty) \leq \sqrt{\gamma_{A,B}}$, and we may relate $\|\rho_{2,2}\|_F$ to $\gamma_{A,B}$ without introducing c_1. Observing that $(1 - \sqrt{\gamma_{A,B}})^2 \leq 1 - \gamma_{A,B}$, we arrive at the first claim. The second follows by observing that $c_3 = 2\sqrt{2 \, \mathrm{cond}(A)}$. $\square$

Notice that one may improve slightly all upper bounds in Theorem 2.3 and Corollary 2.5 (namely, drop each time the first of the two or three terms on the right) if one of the poles $z_{A,j}$ or $z_{B,j}$ is chosen to be ∞ (since then $\rho_{2,2} = 0$). Also, we should mention that each upper bound also implies an upper bound for the error $\|X - X^G_{m,n}\|_F$ by using (1.12). Finally, comparing with Theorem 3.4 it is possible to get upper bounds if one replaces $W(A)$ and $W(B)$ in the definition of $u_{A,m}, u_{B,n}, \gamma_{A,B}, \gamma_{B,A}$ by larger convex sets.

2.4. Comparison with existing work. We have not seen elsewhere in the literature a priori upper bounds for rational Galerkin applied to a Sylvester equation as in Theorem 2.3. Let us therefore compare the findings of Corollary 2.5 for the Lyapunov equation with other results from the literature. In what follows we suppose that A is real, and $\alpha := \lambda_{\min}((A + A^*)/2) > 0$. Also, we denote by ϕ the Riemann map of $W(A)$.

We first have a look at polynomial Galerkin, that is, all $z_{A,j} = z_{B,j} = \infty$. Then $u_{A,n}(z) = 1/|\phi(z)|^n$. Since with $W(A)$ also its level lines (where $|\phi(z)|$ is constant) are convex, we see that the first level line hitting $-W(A)$ passes through $-\alpha$, and thus $\gamma_{A,B} = 1/|\phi(-\alpha)|^n$. Druskin and Simoncini [32, Proposition 3.1] and Kressner and Tobler [25, Corollary 4.4] consider the particular case $A = A^*$, here $\alpha = \lambda_{\min}(A)$, and we find using (2.10) that

$$\gamma_{A,B} = \Big(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \Big)^n \tag{2.11}$$

with

$$\kappa = \frac{\lambda_{\max}(A) + \lambda_{\min}(A)}{2\lambda_{\min}(A)},$$

the same rate of convergence as that found by these authors. However, our constant in front is somehow different. For not necessarily selfadjoint A, if $W(A)$ is included in some ellipse $\mathbb{E}$ then the level lines are explicitly known and $\gamma_{A,B}$ can be computed. In this case we find the rates of convergence of [32, Corollary 4.5] and [25, Theorem 4.8], though it seems that our constants are somehow better. In particular, compared to [24, Remark 3.3] we gain a factor n.

The case of extended Krylov spaces, that is, even n, and half of the poles $z_{A,j}$ being 0 and the other half being ∞, has been discussed in [25, Lemma 6.1] and [24, Section 4] for selfadjoint A. The authors find the rate given in (2.11) with $\kappa = \sqrt{cond(A)}$, in accordance with (2.10). For general A, we have that

$$\gamma_{A,B} = \Big(\max_{z \in -W(A)} \sqrt{\Big| \frac{1}{\phi(z)} \frac{\phi(z) - \phi(0)}{1 - \phi(0)\phi(z)} \Big|} \Big)^n,$$

which at least for disks has been computed in [24, Proposition 5.1]. In the general case the authors show in [24, Theorem 3.2] that the error is bounded by $C\, n\, \gamma_{A,B}$ with a not explicitly given constant C depending on all the data but not on n. We are able to drop this factor n.

Finally, the only result which we are aware of for general rational Galerkin is [16, Proposition 4.5]: for infinite dimensional matrices (operators) A the authors show that the limsup of the nth root of the error is bounded above by the limsup of $[\gamma_{A,B}]^{1/n}$. They conclude in [16, Theorem 4.6 and Proposition 4.7] that if the poles are distributed asymptotically like the equilibrium measure of the condenser consisting of the plates $W(A)$ and $W(-A)$ then the nth root of the error behaves at worst like $R(W(A), W(-A))^{-1}$, where $R(W(A), W(-A))$ is the Riemann modulus of this condenser. This is exactly the classical upper bound for ADI with poles which are optimal for $W(A)$.

We recall the conformal invariance

$$R(W(A), W(-A)) = R(\phi(W(A)), \phi(W(-A))) = R(\mathbb{D}, \phi(W(-A))),$$

the latter being related to some classical well-studied Zolotarev problem. In what follows we use some results from [5, Section 6.2], we refer the reader to the references of that paper for more details. According to [5, Eqn. (6.9)] one has

$$\gamma_{A,B} \geq \frac{1}{R(W(A), W(-A))^n} \tag{2.12}$$

for any choice of the poles.

For the particular case $W(A) \subset (0, \infty)$ a real interval and hence also $\phi(W(-A))$ an (explicitly given) interval $\subset (-\infty, -1)$, one may give an explicit expression of $R(W(A), W(-A))$ in terms of the condition number of A, a formula which involves elliptic integrals. Moreover, it is known that there are poles achieving the lower bound up to a factor 2: according to [5, Proof of Theorem 6.6], one should take as $\phi(z_{A,j}) \in \phi(W(-A))$ the elliptic points of the two intervals $\phi(-W(A)), \phi(-W(A))^{-1}$, that is, the zeros of the explicitly known rational function solving the corresponding Zolotarev problem

$$(2.13)\quad Z_{n,n}(\mathbb{E},\mathbb{F}) := \min_{P,Q\in\mathcal{P}_n} \|\frac{P}{Q}\|_{L^\infty(\mathbb{E})} \|\frac{Q}{P}\|_{L^\infty(\mathbb{F})}, \quad \mathbb{E} = \phi(-W(A)) = \mathbb{F}^{-1}.$$

It is known that this extremal rational function is a Blaschke product, and hence $\gamma_{A,B} = \sqrt{Z_{n,n}(\mathbb{E},\mathbb{F})} \leq 2/R(W(A),W(-A))^n$.

For not necessarily selfadjoint A, in general the shape of $\phi(W(-A))$ might be complicated, and hardly any results on the solution of (2.13) are known. However, "good" poles with small $\gamma_{A,B}$ are obtained by the same principle to choose as $\phi(z_{A,j}) \in \phi(W(-A))$ the zeros of a Blaschke product P/Q giving a small value in (2.13), the choice of poles suggested in [16, Theorem 4.6 and Proposition 4.7].

2.5. Linear versus superlinear convergence. For selfadjoint A, B we have used in this paper the simple upper bound $\|r(A)\| \leq \|r\|_{L^\infty(W(A))}$ for rational functions r. This sometimes severe overestimation might be acceptable for many applications. However, for instance for a cyclic choice of a few multiple poles this leads to upper bounds describing a linear convergence behavior, that is, we consider a "worst case" eigenvalue distribution.

The authors in [3] work instead with discrete maximum norms on $\Lambda(A)$. For sequences of selfadjoint matrices $A = A(N)$ of order N, which for $N \to \infty$ have a joint eigenvalue distribution, they are able to quantify superlinear convergence behavior for the (nth root of the) error after n CG iterations applied to $A(N)$ for $n, N \to \infty$ such that n/N tends to some $t > 0$.

Recently, the asymptotic behavior of rational Ritz values and thus the nth root behavior of $|R_n^G(z)|/\|R_n^G(A)\|$ has been found in [7] in a similar setting, if one supposes in addition that also the sets of poles have some joint distribution (such as a cyclic repetition of few multiple poles). A nice Buyarov–Rakhmanov type formula for this expression in terms of marginal condition numbers can be found in [8]: roughly speaking, instead of $u_{A,m}$ one takes a mean of the formula of $u_{A,m}$ over a family of decreasing sets instead of the fixed set $W(A)$. Inserting these formulas directly in (2.4) allows us to describe superlinear convergence for rational Galerkin applied to a Sylvester or a Lyapunov equation. However, in order to make such a formula more explicit, one has to solve some extremal problems in logarithmic potential theory, involving the asymptotic distribution of eigenvalues and of poles.

In such an (asymptotic) superlinear convergence theory, in order to find optimal poles for ADI or rational Galerkin one should solve (approximately) the discrete Zolotarev problem $Z_{n,n}(\Lambda(A),\Lambda(B))$ instead of the continuous $Z_{n,n}(W(A),W(B))$. The nth root asymptotics for the corresponding optimal rate of convergence can be found in [6].

3. Proofs.

3.1. Proof of Theorem 2.1. For a proof of Theorem 2.1, we need three auxiliary results, which we state each time for $\mathcal{K}_{A,m}$ and for $\mathcal{K}_{B^*,n}$ (however, the second statement follows from the first by taking adjoints). The first and the third property are classical facts for rational Krylov spaces.

The first property is usually referred to as the exactness property of rational Krylov spaces, a proof may be found in [5, Proof of Theorem 5.2] for $z_{A,1} = \infty$, or in [15, Lemma 3.1] for general poles and selfadjoint A. For the sake of completeness we add a proof.

Lemma 3.1. *For any $R_A \in \mathcal{P}_{m-1}/Q_A$ we have that $R_A(A)a = UR_A(A_m)a_m$. Similarly, for any $R_B \in \mathcal{P}_{n-1}/Q_B$ we have that $b^*R_B(B) = b_n^* R_B(B_n)V^*$.*

Proof. By linearity, it is sufficient to consider $R_A(z) = 1/(z-z_j)^\ell \in \mathcal{P}_{m-1}/Q_A$ for some integer $\ell \geq 1$ (and $R_A(z) = z^\ell \in \mathcal{P}_{m-1}/Q_A$ in case $\deg Q_A < m$). By definition of $\mathcal{K}_{A,m}$ and U, there exists a vector $c \in \mathbb{C}^m$ such that

$$R_A(A)a = (A - z_jI)^{-\ell}a = Uc.$$

In case $\ell = 1$ we multiply on the left by $U^*(A - z_jI)$, leading to $a_m = U^*a = U^*(A - z_jI)Uc = (A_m - z_jI)c$, or $c = (A_m - z_jI)^{-1}a_m$, as required. In case $\ell > 1$ we argue by recurrence on ℓ, and obtain $(A_m - z_jI)c = U^*(A - z_jI)^{-\ell+1}a = (A_m - z_jI)^{-\ell+1}a_m$, again as required. The analysis for $R_A(z) = z^\ell$ for $\ell \geq 0$ is similar, we omit details. □

The second property is required for the second part of Theorem 2.1.

Lemma 3.2. *For any $R_A \in \mathcal{P}_m/Q_A$ we have that*

$$(I - \frac{R_A(A)}{R_A(z)})(zI - A)^{-1}a = U(I - \frac{R_A(A_m)}{R_A(z)})(zI - A_m)^{-1}a_m.$$

Similarly, for any $R_B \in \mathcal{P}_n/Q_B$,

$$b^*(zI - B)^{-1}(I - \frac{R_B(B)}{R_B(z)}) = b_n^*(zI - B_n)^{-1}(I - \frac{R_B(B_n)}{R_B(z)})V^*.$$

Proof. It is sufficient to observe that, for fixed z, the function

$$x \mapsto \frac{1 - R_A(x)/R_A(z)}{z - x}$$

is an element of $\mathcal{P}_{m-1}/Q_A$, and to apply Lemma 3.1. □

Our third property is the classical representation of the FOM error for shifted systems in terms of the rational functions (2.1). It follows immediately from Lemma 3.2 by observing that $R_A^G(A_m)a_m = 0$, $b_n^* R_B^G(B_n) = 0$.

Lemma 3.3. *We have that*

$$(zI - A)^{-1}a - U(zI - A_m)^{-1}a_m = \frac{R_A^G(A)}{R_A^G(z)}(zI - A)^{-1}a.$$

Similarly,

$$b^*(zI - B)^{-1} - b_n^*(zI - B_n)^{-1}V^* = b^*(zI - B)^{-1}\frac{R_B^G(B)}{R_B^G(z)}.$$

Proof of the first part of Theorem 2.1. Write shorter $x = (zI - A)^{-1}a$, $\widetilde{x} = (zI - A_n)^{-1}a_n$, $y = b^*(zI - B)^{-1}$, $\widetilde{y} = b_n^*(zI - B_n)^{-1}$, then according to (1.6) and (1.10)

$$X - X_{m,n}^G = \frac{1}{2\pi i}\int_{\Gamma_A}\Big(xy - U\widetilde{x}\widetilde{y}V^*\Big)dz$$

where the compact contour Γ_A encircles once in mathematical positive orientation $\Lambda(A)$ and $\Lambda(A_m)$, but not $\Lambda(B)$ and $\Lambda(B_n)$. We also consider Γ_B, a compact contour encircling once in mathematical positive orientation $\Lambda(B)$ and $\Lambda(B_n)$, but not $\Lambda(A)$ and $\Lambda(A_m)$. Then we can write using Lemma 3.3

$$\begin{aligned} X - X^G_{m,n} &= \frac{1}{2\pi i}\int_{\Gamma_A} \Big((x - U\widetilde{x})y + x(y - \widetilde{y}V^*) - (x - U\widetilde{x})(y - \widetilde{y}V^*) \Big) dz \\ &= \frac{1}{2\pi i}\int_{\Gamma_A} \Big(\frac{R^G_A(A)}{R^G_A(z)} xy + xy \frac{R^G_B(B)}{R^G_B(z)} - \frac{R^G_A(A)}{R^G_A(z)} xy \frac{R^G_B(B)}{R^G_B(z)} \Big) dz. \end{aligned}$$

Let us integrate each term separately. For the first term, observing that the integrand is $\mathcal{O}(z^{-2})_{z\to\infty}$, we replace Γ_A by Γ_B which by the residual theorem gives a change of sign, and thus

$$\begin{aligned} &\frac{1}{2\pi i}\int_{\Gamma_A} \frac{R^G_A(A)}{R^G_A(z)} Axy\, dz - \frac{1}{2\pi i}\int_{\Gamma_A} \frac{R^G_A(A)}{R^G_A(z)} xyB\, dz = I_{1,1} - I_{1,2}, \\ &I_{1,1} := \frac{1}{2\pi i}\int_{\Gamma_B} \frac{R^G_A(A)}{R^G_A(z)} ab^*(zI - B)^{-1}\, dz, \quad I_{1,2} := \frac{1}{2\pi i}\int_{\Gamma_B} \frac{R^G_A(A)}{R^G_A(z)} (zI - A)^{-1}ab^*\, dz, \end{aligned}$$

where, again by the residual theorem, $I_{1,2}$ vanishes.

Similarly, we obtain for the second term the expression $-I_{2,1} + I_{2,2}$, with

$$I_{2,1} := \frac{1}{2\pi i}\int_{\Gamma_A} ab^*(zI - B)^{-1} \frac{R^G_B(B)}{R^G_B(z)}\, dz, \quad I_{2,2} := \frac{1}{2\pi i}\int_{\Gamma_A} (zI - A)^{-1}ab^* \frac{R^G_B(B)}{R^G_B(z)}\, dz,$$

and here the first integral $I_{2,1}$ vanishes by the residual theorem. Finally, for the third term we get $-I_{3,1} + I_{3,2}$, with

$$\begin{aligned} I_{3,1} &:= \frac{1}{2\pi i}\int_{\Gamma_A} \frac{R^G_A(A)}{R^G_A(z)} ab^*(zI - B)^{-1} \frac{R^G_B(B)}{R^G_B(z)}\, dz, \\ I_{3,2} &:= \frac{1}{2\pi i}\int_{\Gamma_A} \frac{R^G_A(A)}{R^G_A(z)} (zI - A)^{-1}ab^* \frac{R^G_B(B)}{R^G_B(z)}\, dz, \end{aligned}$$

where by the residual theorem

$$I_{3,2} = \frac{R^G_A(A)}{R^G_A(\infty)} ab^* \frac{R^G_B(B)}{R^G_B(\infty)} - \frac{1}{2\pi i}\int_{\Gamma_B} \frac{R^G_A(A)}{R^G_A(z)} (zI - A)^{-1}ab^* \frac{R^G_B(B)}{R^G_B(z)}\, dz.$$

By putting the three terms together and applying twice Lemma 3.3, we find that

$$\begin{aligned} &\mathcal{S}_{A,B}(X - X^G_{m,n}) - \frac{R^G_A(A)}{R^G_A(\infty)} ab^* \frac{R^G_B(B)}{R^G_B(\infty)} \\ &= \frac{1}{2\pi i}\int_{\Gamma_B} \frac{R^G_A(A)}{R^G_A(z)} ab^*(zI - B)^{-1}(I - \frac{R^G_B(B)}{R^G_B(z)})\, dz \\ &\quad + \frac{1}{2\pi i}\int_{\Gamma_B} (I - \frac{R^G_A(A)}{R^G_A(z)})(zI - A)^{-1}ab^* \frac{R^G_B(B)}{R^G_B(z)}\, dz \\ &= \frac{1}{2\pi i}\int_{\Gamma_B} \frac{R^G_A(A)}{R^G_A(z)} ab^*_n(zI - B_n)^{-1}V^*\, dz + \frac{1}{2\pi i}\int_{\Gamma_A} U(zI - A_m)^{-1}a_m b^* \frac{R^G_B(B)}{R^G_B(z)}\, dz \\ &= R^G_A(A)ab^*_n \frac{1}{R^G_A}(B_n)V^* + U\frac{1}{R^G_B}(A_m)a_m b^* R^G_B(B), \end{aligned}$$

as claimed in (2.3). Introducing the orthogonal projectors

$$\Pi_A = UU^*, \qquad \Pi_B = VV^*, \tag{3.1}$$

we know from (2.2) that $\Pi_A \rho(I-\Pi_B) = \rho_{1,2}$, $(I-\Pi_A)\rho\Pi_B = \rho_{2,1}$, and $(I-\Pi_A)\rho(I-\Pi_B) = \rho_{2,2}$, from which (2.4) follows. □

Proof of equation (2.5) of Theorem 2.1. For any $R_A \in \mathcal{P}_m/Q_A$ there exists $c_A \in \mathbb{C}$ such that

$$R_A - c_A R_A^G \in \mathcal{P}_{m-1}/Q_A, \quad \frac{c_A}{R_A(\infty)} = \frac{1}{R_A^G(\infty)}.$$

Taking into account the definition of U, (2.2), and Lemma 3.1, we conclude that

$$(I-\Pi_A)\frac{R_A(A)}{R_A(\infty)}a = \frac{R_A^G(A)}{R_A^G(\infty)}a$$

and, similarly, for $R_B \in \mathcal{P}_{n-1}/Q_B$,

$$b^* \frac{R_B(B)}{R_B(\infty)}(I-\Pi_B) = b^* \frac{R_B^G(B)}{R_B^G(\infty)}$$

implying the first part of (2.5). For the second part one has to distinguish two cases: if $R_A^G(\infty) = \infty$ (at least one of the $z_{A,j}$ equals ∞) then $a \in \mathcal{K}_{A,m}$ and the property is trivially true. Otherwise, $\frac{R_A^G(z)}{R_A^G(\infty)} - 1 \in \mathcal{P}_{m-1}/Q_A$ which together with Lemma 3.1 implies that

$$\frac{R_A^G(A)}{R_A^G(\infty)}a = (I-\Pi_A)\frac{R_A^G(A)}{R_A^G(\infty)}a = (I-\Pi_A)a.$$

By the same argument, $b^* \frac{R_B^G(B)}{R_B^G(\infty)} = b^*(I-\Pi_B)$, as claimed in (2.5). □

Proof of equations (2.6), (2.7) of Theorem 2.1. We only show (2.6), the proof of (2.7) is obtained by exchanging the roles of A and B. Since $\rho_{1,2} = \Pi_A \rho(I-\Pi_B)$, we find that $\|\rho_{1,2}\|_F = \|U^*\rho_{1,2}\|_F$. Let us show that, for any $R_B \in \mathcal{P}_n/Q_B$,

$$\|U^*\rho_{1,2}\|_F \le \left\| \frac{1}{R_B}(A_m) a_m b^* R_B(B) \right\|_F + c_0 \left\| \frac{1}{R_B}(A_m) a_m b_n^* R_B(B_n) \right\|_F. \tag{3.2}$$

Since $R_B^G(B_n) = 0$ by (2.1), we see from (2.3) that there is equality in (3.2) for $R_B = R_B^G$, and hence (2.6) follows.

We have

$$\begin{aligned}
U^*\rho_{1,2} &= \frac{1}{R_B^G}(A_m)a_m b^* R_B^G(B) = \frac{1}{2\pi i}\int_{\Gamma_A} (zI-A_m)^{-1} a_m b^* \frac{R_B^G(B)}{R_B^G(z)}\, dz \\
&= \frac{1}{2\pi i}\int_{\Gamma_A} (zI-A_m)^{-1} a_m \Big(b^*(zI-B)^{-1} - b_n^*(zI-B_n)^{-1}V^* \Big)(zI-B)\, dz \\
&= I_1 - I_2, \\
I_1 &:= \frac{1}{2\pi i}\int_{\Gamma_A} (zI-A_m)^{-1} a_m \Big(b^*(zI-B)^{-1} \frac{R_B(B)}{R_B(z)} \Big)(zI-B)\, dz, \\
I_2 &:= \frac{1}{2\pi i}\int_{\Gamma_A} (zI-A_m)^{-1} a_m \Big(b_n^*(zI-B_n)^{-1} \frac{R_B(B_n)}{R_B(z)} V^* \Big)(zI-B)\, dz,
\end{aligned}$$

where we have applied first Lemma 3.3 and then Lemma 3.2. Notice that if one of the roots of R_B coincides with one of the eigenvalues of A_m then we adapt the convention that $\|\frac{1}{R_B}(A_m)\|$ has norm ∞. Otherwise, we may deform Γ_A such that it encircles $\Lambda(A_m)$ but not the roots of R_B. In this case, $I_1 = \frac{1}{R_B}(A_m)a_m b^* R_B(B)$, and it remains to show that

$$\|I_2\|_F \leq c_0 \, \| \frac{1}{R_B}(A_m) a_m b_n^* R_B(B_n) \|_F. \tag{3.3}$$

By (1.10) and the Cauchy residual formula,

$$\begin{aligned}
\mathcal{S}_{A_m,B}^{-1} I_2 &= \frac{1}{2\pi i} \int_{\Gamma_B} (\zeta I - A_m)^{-1} \frac{1}{2\pi i} \int_{\Gamma_A} (zI - A_m)^{-1} a_m \\
&\qquad \Big(b_n^* (zI - B_n)^{-1} \frac{R_B(B_n)}{R_B(z)} V^* \Big) (zI - B) \, dz \, (\zeta I - B)^{-1} \, d\zeta \\
&= \frac{1}{2\pi i} \int_{\Gamma_B} (\zeta I - A_m)^{-1} \frac{1}{2\pi i} \int_{\Gamma_A} (zI - A_m)^{-1} a_m \\
&\qquad \Big(b_n^* (zI - B_n)^{-1} \frac{R_B(B_n)}{R_B(z)} V^* \Big) (z - \zeta) \, dz \, (\zeta I - B)^{-1} \, d\zeta \\
&= \frac{1}{2\pi i} \int_{\Gamma_B} \frac{1}{2\pi i} \int_{\Gamma_A} \Big((\zeta I - A_m)^{-1} - (zI - A_m)^{-1} \Big) a_m \\
&\qquad \Big(b_n^* (zI - B_n)^{-1} \frac{R_B(B_n)}{R_B(z)} V^* \Big) \, dz \, (\zeta I - B)^{-1} \, d\zeta \\
&= -\frac{1}{2\pi i} \int_{\Gamma_A} (zI - A_m)^{-1} a_m b_n^* (zI - B_n)^{-1} \frac{R_B(B_n)}{R_B(z)} V^* \, dz.
\end{aligned}$$

As above we deduce that

$$\begin{aligned}
\mathcal{S}_{A_m,B_n} \Big(\mathcal{S}_{A_m,B}^{-1} I_2 \Big) &= -\frac{1}{2\pi i} \int_{\Gamma_A} (zI - A_m)^{-1} a_m b_n^* \frac{R_B(B_n)}{R_B(z)} V^* \, dz \\
&= -\frac{1}{R_B}(A_m) a_m b_n^* R_B(B_n) V^*.
\end{aligned}$$

Hence

$$\|I_2\|_F \leq \|\mathcal{S}_{A_m,B_n}^{-1}\| \, \|\mathcal{S}_{A_m,B}\| \, \| \frac{1}{R_B}(A_m) a_m b_n^* R_B(B_n) \|_F,$$

and our claim (3.3) follows from (1.11) and (1.12). □

3.2. Proof of Corollary 2.2. Comparing (1.3) with Theorem 2.1 for $m = n$, we may choose $R^{ADI} = R_B = 1/R_A$ in (2.5), (2.6), and (2.7).

Then $R_A(\infty) R_B(\infty) = 1$, and thus by (2.5)

$$\|\rho_{2,2}\|_F \leq \|R_A(A) a b^* R_B(B)\|_F = \|\mathcal{S}_{A,B}(X - X_n^{ADI})\|_F.$$

For the upper bound for $\|\rho_{1,2}\|$ given in (2.6), we first observe that $R_A - \frac{R_A^G}{R_A^G(\infty)} \in \mathcal{P}_{m-1}/Q_A$, and hence by Lemma 3.1, (2.1), (2.2), and (3.1),

$$\Pi_A R_A(A) a = U U^* R_A(A) a = U R_A(A_n) a_n,$$

and similarly $b^* R_B(B)\Pi_B = b_n^* R_B(B_n) V^*$. Hence by (2.6)

$$\begin{aligned}\|\rho_{1,2}\|_F &\le \|R_A(A_n)a_n b^* R_B(B)\|_F + c_0 \,\|R_A(A_n)a_n b_n^* R_B(B_n)\|_F \\ &\le (1+c_0)\,\|\mathcal{S}_{A,B}(X - X_n^{ADI})\|_F.\end{aligned}$$

The same conclusion is obtained for $\|\rho_{2,1}\|$, and thus Corollary 2.2 holds.

3.3. Proof of Theorem 2.3. We start by giving a result related to the extremal quantities $E(A, Q_A, z)$ and $E(W(A), Q_A, z)$ defined in (2.8), and (2.9), respectively. In our proof of Theorem 3.4 we do not use field–of–value estimates of Crouzeix [13], but merely generalize the techniques from [4].

THEOREM 3.4. *Let $\mathbb{E} \subset \mathbb{C}$ be some convex compact set (not a single point), and A a square matrix with $W(A) \subset \mathbb{E}$. For all $R_A \in \mathcal{P}_m/Q_A$ and for all $z \notin \mathbb{E}$*

$$\frac{\|R_A\|_{L^\infty(\mathbb{E})}}{|R_A(z)|} \ge u(z) := \exp\Big(-\sum_{j=1}^m g(z, z_{A,j})\Big),$$

with $g(\cdot,\zeta)$ the Green function of $\mathbb{C}\setminus\mathbb{E}$ with pole at ζ. This inequality is sharp up to some modest constant in the sense that there exists $R_A^\# \in \mathcal{P}_m/Q_A$ having m zeros in $\mathbb{E}$ with

$$\begin{aligned}&\|R_A^\#\|_{L^\infty(\mathbb{E})} \le 2, \quad \|R_A^\#(A)\| \le 2, \\ &\forall z \notin \mathbb{E}: \quad \frac{1}{|R_A^\#(z)|} \le \frac{u(z)}{1-u(z)}.\end{aligned}$$

Proof. The first inequality is known as the rational version of the Bernstein–Walsh inequality due to Gonchar [23]. For a proof, it is sufficient to notice that the function $f(z) = \log|R_A(z)\,u(z)|$ is subharmonic in $\mathbb{C}\setminus\mathbb{E}$, and to apply the maximum principle for subharmonic functions, leading to $f(z) \le \|f\|_{L^\infty(\partial\mathbb{E})} \le \|\log|R_A|\,\|_{L^\infty(\mathbb{E})}$.

For showing the second part, we denote by ϕ the Riemann conformal mapping of $\mathbb{C}\setminus\mathbb{E}$ onto $\mathbb{C}\setminus\mathbb{D}$, $\mathbb{D}$ the closed unit disk, with $\phi(\infty) = \infty$ and $\phi'(\infty) > 0$. Also, denote the inverse map by $\psi = \phi^{-1}$. If all $z_{A,j} \in \mathbb{E}$, then $u(z) = 1$ (all Green functions vanish), and the second statement is trivially true. Otherwise, we may choose $R_A^\#$ by prescribing as roots all $z_{A,j} \in \mathbb{E}$. Since the corresponding terms in u vanish, we may suppose without loss of generality for our construction of $R_A^\#$ that all roots $z_{A,j}$ of Q_A are outside $\mathbb{E}$. Then it is known that one can write the function u in terms of Blaschke products

$$\frac{1}{u(z)} = |h(\phi(z))|, \quad h(w) = \prod_{j=1}^m \frac{1 - \overline{\phi(z_{A,j})}w}{w - \phi(z_{A,j})}.$$

Notice that h is analytic in $\mathbb{D}$, and meromorphic outside of $\mathbb{D}$.

The Faber map $\mathcal{F}$ identifies functions analytic in $\mathbb{D}$ with functions analytic in $\mathbb{E}$ via the formula

$$z \in \mathrm{Int}(\mathbb{E}): \quad \mathcal{F}(p)(z) = \int_{|w|=1} p(w) \frac{w\psi'(w)}{\psi(w) - z} \frac{dw}{2\pi i w},$$

in particular $\mathcal{F}(\mathcal{P}_m) = \mathcal{P}_m$, and $\mathcal{F}(\mathcal{P}_m/Q) = \mathcal{P}_m/Q_A$, with $Q(z) = \prod_{j=1}^m (w - \phi(z_{A,j}))$, see for instance [5] and the references therein. In particular,

$$R_A^\#(z) := \mathcal{F}(h)(z) + h(0) \in \mathcal{P}_m/Q_A.$$

By deforming the path of integration towards ∞ we also see that

$$\int_{|w|=1} \overline{h(w)} \frac{w\psi'(w)}{\psi(w)-z} \frac{dw}{2\pi i w} = \int_{|w|=1} \frac{1}{h(w)} \frac{w\psi'(w)}{\psi(w)-z} \frac{dw}{2\pi i w} = \frac{1}{h(\infty)} = \overline{h(0)}$$

since $1/h$ is analytic outside $\mathbb{D}$. Thus

$$R_A^{\#}(z) = \int_{|w|=1} h(w) \mathrm{Re}\Big(2 \frac{w\psi'(w)}{\psi(w)-z}\Big) \frac{dw}{2\pi i w}. \tag{3.4}$$

Since the real part is positive for all $z \in \mathrm{Int}(\mathbb{E})$, we obtain

$$\|R_A^{\#}\|_{L^\infty(\mathbb{E})} \le \|h\|_{L^\infty(\mathbb{D})} \sup_{z\in \mathrm{Int}(\mathbb{E})} \int_{|w|=1} \mathrm{Re}\Big(2 \frac{w\psi'(w)}{\psi(w)-z}\Big) \frac{dw}{2\pi i w} = 2.$$

As explained in more detail, e.g., in [5, Proof of Theorem 2.1], the above reasoning remains true after replacing the scalar argument z by the matrix A, leading to the similar conclusion $\|R_A^{\#}(A)\| \le 2$. Finally, for $|v| < 1$, we have the Poisson kernel formula

$$h(v) = \int_{|w|=1} h(w) \mathrm{Re}\Big(\frac{w+v}{w-v}\Big) \frac{dw}{2\pi i w}, \tag{3.5}$$

which can also be shown directly as in (3.4). The above convexity argument shows that

$$\mathrm{Re}\Big(2 \frac{w\psi'(w)}{\psi(w)-\psi(v)} - \frac{w+v}{w-v}\Big)$$

is ≥ 0 for $|v| = 1 = |w|$, $v \ne w$, and thus also for $|v|, |w| \ge 1$ by the maximum principle. Combining the two integrals (3.4) and (3.5), we conclude that

$$\|R_A^{\#} \circ \psi - h\|_{L^\infty(\mathbb{D})} \le \lim_{\epsilon\to 0} \sup_{|v|=1} \int_{|w|=1+\epsilon} \mathrm{Re}\Big(2 \frac{w\psi'(w)}{\psi(w)-\psi(v)} - \frac{w+v}{w-v}\Big) \frac{dw}{2\pi i w} \le 1.$$

Finally, the maximum principle applied to the function $v \mapsto R_A^{\#}(\psi(v)) - h(v)$ analytic in $\overline{\mathbb{C}} \setminus \mathbb{D}$ tells us that, for all $z \notin \mathbb{E}$,

$$|R_A^{\#}(z)| \ge |h(\phi(z))| - 1 = \frac{1}{u(z)} - 1 > 0,$$

as required for the assertion of Theorem 3.4. □

We learn from Theorem 3.4 that, for convex compact $\mathbb{E}$ and for matrices A with $W(A) \subset \mathbb{E}$, $z \notin \mathbb{E}$,

$$1 \le \frac{E_m(\mathbb{E}, Q_A, z)}{u(z)} \le \frac{2}{1-u(z)}, \qquad \frac{E_m(A, Q_A, z)}{u(z)} \le \frac{2}{1-u(z)},$$

where we may construct (diagonal) matrices A with $E_m(A, Q_A, z) \le E_m(\mathbb{E}, Q_A, z)$ arbitrarily close to $E_m(\mathbb{E}, Q_A, z)$. In the particular case $Q_A = 1$ and thus $z_{A,1} = ... = z_{A,m} = \infty$, our assertion reduces to

$$1 \le \frac{E_m(\mathbb{E}, 1, z)}{|\phi(z)|^{-m}} \le \frac{2}{1-|\phi(z)|^{-m}}, \qquad \frac{E_m(A, 1, z)}{|\phi(z)|^{-m}} \le \frac{2}{1-|\phi(z)|^{-m}},$$

the left–hand inequality being known as the classical Bernstein–Walsh inequality. With the notations of the proof of Theorem 3.4, we get $h(w) = w^m$, and hence $R_A^{\#}(z) = \mathcal{F}(w^m)(z) = F_m(z)$, the mth Faber polynomial. The inequalities $\|F_n(A)\| \leq 2$ and the slight improvement $E_m(A, 1, z) \leq 2|\phi(z)|^{-m}/(1 - |\phi(z)|^{-m-1})$ have been established already in [4, Théorème 1 and Théorème 2].

The following example shows that, in special cases, we have even found the solution of the extremal problem $E_m(\mathbb{E}, Q_A, z)$.

Example 3.5. *For the particular case of $\mathbb{E} = [\alpha, \beta]$ a real interval (and hence A selfadjoint), $z \in \mathbb{R} \setminus \mathbb{E}$, and $\{z_{A,1}, ..., z_{A,m}\}$ closed under complex conjugation, it is known that, for $|w| \geq 1$,*

$$\psi(w) = \frac{\beta + \alpha}{2} + \frac{\beta - \alpha}{2}\frac{w + w^{-1}}{2}, \quad \mathcal{F}(P)(\psi(w)) = P(w) + P(\frac{1}{w}) - P(0).$$

Hence here, for $|w| \geq 1$,

$$R_A^{\#}(\psi(w)) = h(w) + h(\frac{1}{w}) = h(w) + \overline{1/h(\overline{w})},$$

and it is not difficult to see that $\|R_A^{\#}\|_{L^\infty(\mathbb{E})} = 2$ and, more precisely, $R_A^{\#}$ has the alternation property of oscillating $m + 1$ times between the values ± 2 on $\mathbb{E}$. One may deduce [26] that $R_A^{\#}$ is the extremal function of the extremal problem $E_m([\alpha, \beta], Q_A, z)$ for $z \in \mathbb{R} \setminus [\alpha, \beta]$, i.e.,

$$\frac{E_m([\alpha, \beta], Q_A, z)}{u(z)} = \frac{2}{u(z)|R_A^{\#}(z)|} = \frac{2}{1 + u(z)^2} \in [1, 2].$$

Hence it is quite unlikely that Theorem 3.4 can be essentially improved, even for selfadjoint A. □

We are now prepared to proceed with our proof.

Proof of Theorem 2.3 for general A, B. Since $W(A_m) \subset W(A)$, $W(B_n) \subset W(B)$, each of the terms occurring in equations (2.5), (2.6), and (2.7) of Theorem 2.1 can be bounded from above in terms of (2.8), Theorem 3.4, and the field–of value estimate of Crouzeix.

For (2.6), taking into account that the matrix ab^* is of rank 1, we have that

$$\begin{aligned}\frac{\|\rho_{1,2}\|_F}{\|a\|\,\|b\|} &\leq \min_{R_B \in \frac{\mathcal{P}_n}{Q_B}} \frac{\|\frac{1}{R_B}(A_m)a_m\|}{\|a\|}\frac{\|b^* R_B(B)\|}{\|b\|} + c_0 \frac{\|\frac{1}{R_B}(A_m)a_m\|}{\|a\|}\frac{\|b_n^* R_B(B_n)\|}{\|b\|} \\ &\leq C_{Crouzeix}\,(1 + c_0) \max_{z \in W(A)} \frac{2\,u_{B,n}(z)}{1 - u_{B,n}(z)} = C_{Crouzeix}\,(1 + c_0)\,\frac{2\gamma_{B,A}}{1 - \gamma_{B,A}},\end{aligned}$$

and similarly

$$\frac{\|\rho_{2,1}\|_F}{\|a\|\,\|b\|} \leq C_{Crouzeix}\,(1 + c_0)\,\frac{2\,\gamma_{A,B}}{1 - \gamma_{A,B}}.$$

For (2.5) we obtain

$$\frac{\|\rho_{2,2}\|_F}{\|a\|\,\|b\|} \leq \inf_{\substack{R_A \in \frac{\mathcal{P}_m}{Q_A} \\ R_B \in \frac{\mathcal{P}_n}{Q_B}}} \frac{\|R_A(A)a\|\,\|b^* R_B(B)\|}{\|a\|\|b\||R_A(\infty)R_B(\infty)|} \tag{3.6}$$

$$
\begin{aligned}
&\leq E_m(W(A), Q_A, \infty)\, E_n(W(B), Q_B, \infty) \\
&\leq \frac{2\, u_{A,m}(\infty)}{1 - u_{A,m}(\infty)} \frac{2\, u_{B,n}(\infty)}{1 - u_{B,n}(\infty)}. \\
&\leq 4\, c_1\, u_{A,m}(\infty)\, u_{B,n}(\infty),
\end{aligned}
$$

the last inequality following immediately from the definition of $c_1, u_{A,m}, u_{B,n}$ by taking into account that Green functions are nonnegative. In order to relate this last quantity to $\max\{\gamma_{A,B}, \gamma_{B,A}\} < 1$, we notice that $z \mapsto \log(u_{A,m}(z) u_{B,n}(z))$ is subharmonic in $\mathbb{C} \setminus (W(A) \cup W(B))$. Hence using the maximum principle

$$
\log(u_{A,m}(\infty) u_{B,n}(\infty)) \leq \max_{z \in W(A) \cup W(B)} \log(u_{A,m}(z) u_{B,n}(z))
$$

$$
= \log \max\Big\{ \max_{z \in W(B)} u_{A,m}(z),\ \max_{z \in W(A)} u_{B,n}(z) \Big\} = \log \max\{\gamma_{A,B}, \gamma_{B,A}\}.
$$

Thus we have established the first estimate of Theorem 2.3. □

Proof of Theorem 2.3 for selfadjoint A, B. We closely follow the proof above, but here we may slightly change some arguments in order to improve our constants. By assumption, $W(A), W(B)$ are disjoint real intervals, and we may suppose without loss of generality that $W(A)$ lies on the left of $W(B)$ (otherwise we pass to the adjoint equation).

First of all, from Example 3.5 we have the slightly sharper bounds

$$
\begin{aligned}
E_m(A, Q_A, z) &\leq E_m(W(A), Q_A, z) \leq 2\, u_{A,m}(z), \\
E_n(B, Q_B, z) &\leq E_n(W(B), Q_B, z) \leq 2\, u_{B,n}(z).
\end{aligned}
$$

Comparing with the above proof, we may therefore drop the constant c_1 and conclude that $\|\rho_{2,2}\|_F \leq 4 \max\{\gamma_{A,B}, \gamma_{B,A}\}$.

Concerning $\|\rho_{2,1}\|_F$, we will return to the proof of Theorem 2.1 since on the real line we may exploit another extremal property, namely that the nth orthogonal polynomial for some discrete measure is a kernel polynomial of a modified measure, and hence solution of some L^2 extremal problem.

Write more explicitly $R_A^G(z) = p_m(z)/Q_A(z)$, then (2.2) tells us that, for all $p \in \mathcal{P}_{m-1}$,

$$
\int \overline{p(z)} p_m(z)\, d\mu(z) = 0, \qquad \int \overline{P} Q\, d\mu := [\frac{P}{Q_A}(A)a]^* \frac{Q}{Q_A}(A)a
$$

and hence p_m is a monic mth orthogonal polynomial with respect to the positive discrete measure μ with real support $\subset \Lambda(A)$. Consider now for some $\sigma > \lambda_{\max}(A)$ the modified positive measure $d\nu(x) = d\mu(x)/(\sigma - x)$, together with the orthonormal polynomials $q_0, ..., q_{m+1}$. Then $q_{m+1}(z) - q_m(z) q_{m+1}(\sigma)/q_m(\sigma) = (z - \sigma) q(z)$ for some $q \in \mathcal{P}_m$. The ν–orthogonality conditions for $(z - \sigma)q(z)$ allow us to conclude that q is μ–orthogonal to $\mathcal{P}_{m-1}$ and hence a non–trivial multiple of p_m. Taking into account the Rodriguez formula for orthogonality on the real line, we conclude that $p_n(z)$ is a non–trivial multiple of the kernel polynomial

$$
\sum_{j=0}^{m} q_j(\sigma) q_j(z).
$$

Since this latter is known to be extremal, we conclude that

$$
\min_{p \in \mathcal{P}_m} \frac{\int |p(z)|^2\, d\nu(z)}{|p(\sigma)|^2} = \frac{\int |p_m(z)|^2\, d\nu(z)}{|p_m(\sigma)|^2} = \frac{\int |p_m(z)|^2\, \frac{d\mu(z)}{\sigma - z}}{|p_m(\sigma)|^2}.
$$

In terms of linear algebra, this implies that

$$\begin{aligned}
&\frac{1}{\sigma-\lambda_{\min}(A)}\frac{\|R_A^G(A)a\|^2}{|R_A^G(\sigma)|^2} \leq \frac{(R_A^G(A)a)^*(\sigma I-A)^{-1}R_A^G(A)a}{|R_A^G(\sigma)|^2} \\
&= \min_{R_A\in\mathcal{P}_m/Q_A} \frac{(R_A(A)a)^*(\sigma I-A)^{-1}R_A(A)a}{|R_A(\sigma)|^2} \\
&\leq \frac{\|a\|^2}{\sigma-\lambda_{\max}(A)}E_m(A,Q_A,\sigma)^2.
\end{aligned}$$

Hence by (2.3)

$$\begin{aligned}
\Big(\frac{\|\rho_{2,1}\|_F}{\|a\|\,\|b\|}\Big)^2 &\leq \Big(\frac{\|R_A^G(A)ab_n^*\frac{1}{R_A^G}(B_n)\|_F}{\|a\|\,\|b\|}\Big)^2 \\
&\leq \max_{\sigma\in\Lambda(B_n)} \frac{\|R_A^G(A)a\|^2}{\|a\|^2\,|R_A^G(\sigma)|^2} \\
&\leq \max_{\lambda\in\Lambda(B_n)} \frac{\lambda-\lambda_{\min}(A)}{\lambda-\lambda_{\max}(A)} \max_{\sigma\in\Lambda(B_n)} E_m(A,Q_A,\sigma)^2 \\
&\leq 4\,\frac{\lambda_{\min}(B)-\lambda_{\min}(A)}{\lambda_{\min}(B)-\lambda_{\max}(A)}\,\gamma_{A,B}^2
\end{aligned}$$

and similarly

$$\Big(\frac{\|\rho_{1,2}\|_F}{\|a\|\,\|b\|}\Big)^2 \leq 4\,\frac{\lambda_{\max}(B)-\lambda_{\max}(A)}{\lambda_{\min}(B)-\lambda_{\max}(A)}\,\gamma_{B,A}^2.$$

Thus our claimed estimate follows from (2.4). □

The arguments used in the second part of the preceding proof can also be used to show that, for systems of equations with a Hermitian positive definite matrix of coefficients, the FOM method is mathematically equivalent to CG. Indeed, Kressner and Tobler in [25, Section 4.1] used for the Lyapunov equation an expression reminding of the A–norm of the error of CG, by exploiting bivariate polynomial extremal problems.

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