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A GMRES CONVERGENCE ANALYSIS FOR LOCALIZED INVARIANT SUBSPACE ILL-CONDITIONING*

GIULIA SACCHI† AND VALERIA SIMONCINI†

Abstract. The Generalized Minimal RESidual (GMRES) method is a well-established strategy for iteratively solving a large linear system $Ax = b$, where $A \in \mathbb{R}^{n\times n}$ is a nonsymmetric and nonsingular coefficient matrix, and $b \in \mathbb{R}^n$. In the analysis of its convergence for A diagonalizable, a much used upper bound for the relative residual norm involves a min-max polynomial problem over the set of eigenvalues of A, magnified by the condition number of the eigenvector matrix of A. This latter factor may cause a huge overestimation of the residual norm, making the bound nondescriptive in practice. We show that when a large condition number is caused by the almost linear dependence of a few of the eigenvectors, a more descriptive analysis of the method's behavior can be performed, irrespective of the location of the corresponding eigenvalues. The new analysis aims at capturing how the GMRES polynomial deals with the ill-conditioning; as a by-product, a new upper bound for the GMRES residual norm is obtained. A variety of numerical experiments illustrate our findings.

Key words. GMRES, min-max polynomial problem, GMRES convergence, residual norm minimization

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1. Introduction.

The Generalized Minimal RESidual (GMRES) [23] method is a well-established and particularly effective strategy for iteratively solving a large linear system

$$Ax = b,$$

where $A \in \mathbb{R}^{n\times n}$ is a nonsymmetric and nonsingular coefficient matrix, $b \in \mathbb{R}^n$ is the right-hand side, and n is very large, say $n = \mathcal{O}(10^6)$ or greater. This projection-type method is optimal in the sense that at each iteration it minimizes the residual norm over all possible approximate solutions belonging to the approximation space. More precisely, given a starting approximate solution $x_0 \in \mathbb{R}^n$ and the associated residual $r_0 = b - Ax_0$, after m iterations the method has generated the Krylov subspace $K_m(A, r_0) = \text{span}\{r_0, Ar_0, \ldots, A^{m-1}r_0\}$ and an approximate solution x_m such that

$$x_m = \arg \min_{x\in x_0+K_m(A,r_0)} \|b - Ax\|.$$

Over the years, analysis of GMRES convergence has attracted the interest of many researchers, giving rise to a rich and particularly deep literature; see, e.g., [16] for a recent account. Although we have a good understanding of GMRES behavior in special settings, such as when A is normal (see, e.g., [17]), available general a priori convergence estimates still are not always descriptive of the actual behavior of the method [7]. For A diagonalizable, let $A = X\Lambda X^{-1}$, where X is the eigenvector

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†Dipartimento di Matematica, Università di Bologna, Piazza di Porta S. Donato, 5, I-40127 Bologna, Italy (giulia.sacchi3@studio.unibo.it, valeria.simoncini@unibo.it).

matrix and $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$, with λ_j, $j = 1, \ldots, n$, eigenvalues of A. The most well known bound for the norm of the residual $r_m = b - Ax_m$ is given by

$$\frac{\|r_m\|}{\|r_0\|} \le \kappa(X) \min_{p \in \mathbb{P}_m^*} \max_{k=1,\ldots,n} |p(\lambda_k)|, \tag{1.1}$$

where $\kappa(X) = \|X\| \, \|X^{-1}\|$ is the condition number of X in the matrix norm induced by the Euclidean vector norm, and $\mathbb{P}_m^*$ is the set of comonic[1] polynomials. Even when the min-max problem accurately captures the true decay of the residual norm as the iterations proceed, a large value of $\kappa(X)$ may unrealistically increase the gap between the bound and the residual norm. In [14] it was explicitly observed that by extracting $\kappa(X)$ from the min-max problem, a beneficial cancellation taking place in the actual residual—as a linear combination of eigenvectors of A—is lost; we also refer the reader to the detailed discussion in [7] on different ways to represent the residual in terms of spectral components of A. In [15] the authors thus employ a well-conditioned transformation for a class of discretization methods for certain convection-diffusion problems that allows them to isolate the ill-conditioning of their specific problem within a block diagonal matrix. The idea of isolating the bad and good invariant subspaces has been used in other contexts (see, e.g., [2]), and the transformation is effective if a priori spectral information is available. Here we start by an explicit formulation of the ill-conditioning, and in section 5 we expand on this idea for general diagonalizable matrices by first determining a unitary transformation that can detect —if present—the localized ill-conditioning of the given eigenvector matrix.

The inclusion of $\kappa(X)$ in (1.1) may make the upper bound too pessimistic—to the point that quantities other than the eigenpairs, such as the field of values or the pseudospectrum of A, have been used to obtain more descriptive upper bounds; see, e.g., [11], [3], [12], [20], [13], [28], [29]. The role of the right-hand side and the use of well-conditioned transformations for a particular class of problems have been discussed in [15]. We refer the reader to [27] for a survey of different tools used in this context. Other bounds addressing special cases, such as outlying eigenvalues, have been proposed; see, e.g., [4].

On the one hand, it is possible to construct problems where intrinsic ill-conditioning of the whole eigenbasis X has dramatic effects. On the other hand, it sometimes happens that ill-conditioning of X is due to just a small number of its columns. Identifying and isolating the invariant spaces responsible for ill-conditioning may lead to a more accurate description of the GMRES convergence. Our aim is to introduce a new GMRES convergence analysis for diagonalizable coefficient matrices that addresses the case of localized invariant subspace ill-conditioning. In this setting, the ill-conditioned portion of X is retained in the polynomial minimization problem, and its effect on the polynomial problem is accounted for by including an appropriate constraint in the minimization problem. Our numerical experience seems to show that this strategy is particularly close to what the GMRES polynomial actually does to deal with this form of ill-conditioning. We emphasize that we are interested in the behavior of the complete eigenvector basis, and thus we restrict ourselves to diagonalizable matrices, except for a short digression in section 3 where certain Jordan matrices are discussed for comparison purposes.

The idea of isolating the "bad" invariant subspace in GMRES has already been explored in [6] to describe the GMRES behavior when the matrix A is close to singular due to a relatively small group of eigenvalues located in a neighborhood of zero. The

[1] A comonic polynomial p is such that $p(0) = 1$.

situation there is rather different than in our case. In [6], the ill-posed problem context allows one to split A into its far-from-singular and almost-singular parts and focus on the former (noise-free) part.

In our setting no invariant subspace can be neglected, and our analysis focuses on the relation between invariant subspaces of A and their influence on the convergence. Thus we keep in mind that eigenvalues alone may not be sufficient to describe the GMRES behavior [11], [10], [1], [16]. In particular, we stress that our analysis does not rely on the ill-conditioned eigenvalues having particular geometric properties, such as being outliers or clustered, and in fact, the eigenvalue location is largely irrelevant, as long as A is far from singular. Nonetheless, the relation between our estimate and the occurrence of Jordan blocks is also explored.

In our convergence analysis the original GMRES polynomial minimization problem is bounded by means of a modest multiple of a *constrained* polynomial min-max problem over the set of eigenvalues, where the constraint is used to balance the polynomial growth in the neighborhood of eigenvalues associated with almost linearly dependent eigenvectors. With our analysis we claim that to minimize the residual norm in correspondence to the ill-conditioned portion of the eigenvector matrix, the GMRES residual polynomial should take almost the same values at the associated eigenvalues; this requirement gives rise to a *constraint* for the polynomial minimization problem, which seems to hold in practice for the computed GMRES residual polynomial. A variety of numerical experiments, some of which were reported in [24], seem to support the high fidelity of the new bounds.

A synopsis of the paper is as follows. First, we focus on the simpler situation in which just two eigenvectors are almost parallel by presenting a convergence analysis in section 2 and its subsections, followed by a comparison analysis with the occurrence of a Jordan block matrix in section 3. In section 4, we propose a convergence analysis for two close invariant subspaces, associated to generally different eigenvalues. Finally, in section 5 we address the situation where the ill-conditioning localization is not known a priori, and we show how our methodology can be adapted to this setting.

All experiments were performed in MATLAB [18]. Whenever needed for numerical illustration, the constrained optimization problem was solved as discussed in the appendix.

2. Two-dimensional ill-conditioning.

2.1. The ill-conditioning model. Let us consider the unitary matrix

$$\widehat{X} := [\widehat{x}_1, \widehat{x}_2, \widehat{x}_3, \dots, \widehat{x}_n] \in \mathbb{C}^{n\times n}$$

and, for $\varepsilon > 0$, the matrix X defined as

$$X := \widehat{X} \begin{bmatrix} \begin{pmatrix} 1 & 1 \\ & \varepsilon \end{pmatrix} & \\ & I_{n-2} \end{bmatrix} = [\widehat{x}_1, \widehat{x}_1 + \varepsilon\widehat{x}_2, \widehat{x}_3, \dots, \widehat{x}_n], \tag{2.1}$$

where I_{n-2} is the $(n-2)\times(n-2)$ identity matrix. For $\lambda_i \in \mathbb{C}$, $i = 1, \dots, n$, let $A = X\Lambda X^{-1}$ be a (diagonalizable) matrix having X as the eigenvector matrix and $\Lambda :=\text{diag}(\lambda_1, \dots, \lambda_n)$ as the eigenvalue matrix. For the sake of convenience we single out the first two (distinct) eigenvalues as

$$\alpha := \lambda_1, \quad \beta := \lambda_2.$$

Then we can write

$$A = X\Lambda X^{-1} = \widehat{X} L \widehat{X}^H, \tag{2.2}$$

where $L = \text{blkdiag}(L_1, L_2)$ with

$$L_1 = \begin{bmatrix} 1 & 1 \\ & \varepsilon \end{bmatrix} \begin{bmatrix} \alpha & 0 \\ 0 & \beta \end{bmatrix} \begin{bmatrix} 1 & 1 \\ & \varepsilon \end{bmatrix}^{-1} = \begin{bmatrix} \alpha & \frac{\beta-\alpha}{\varepsilon} \\ 0 & \beta \end{bmatrix}, \qquad L_2 := \text{diag}(\lambda_3, \dots, \lambda_n). \tag{2.3}$$

The matrix A is almost normal; its nonnormality is due to the eigenvectors associated with α, β, which are close to being linearly dependent for small ε. A similar example was used in [11], where the fact that eigenvalue information alone cannot predict the actual GMRES convergence is deeply investigated.

Assumption 2.1. *Throughout the paper we assume that α and β are* distinct *and can be far apart. Hence, in the case when we write $|\alpha - \beta| \to 0$ we mean that α and β are in a neighborhood of each other but remain distinct.*

Let $\kappa(\lambda) = \frac{1}{|y^H x|}$ be the eigenvalue condition number of λ, where x and y are its right and left unit eigenvectors, respectively. With the definition in (2.3), A has two ill-conditioned eigenvalues, namely α and β, whose conditioning blows up as ε tends to zero. More precisely, the following result holds.

Proposition 2.2. *Let α, β be the eigenvalues of the matrix A defined in* (2.2)*. Then $\kappa(\alpha) = \kappa(\beta) = \sqrt{1 + \frac{1}{\varepsilon^2}}$.*

Proof. The eigenvalues α and β have right eigenvectors $x_1 = \widehat{x}_1$ and $x_2 = \widehat{x}_1 + \varepsilon\widehat{x}_2$, respectively. The unnormalized matrix of left eigenvectors of A is given by $Y = [Y_1, Y_2] = X^{-H}$, so that its block of the first two vectors satisfies $Y_1 = [y_1, y_2] = \widehat{X}_1 V^{-H}$, with

$$\widehat{X}_1 := [\widehat{x}_1, \widehat{x}_2], \qquad V := \begin{bmatrix} 1 & 1 \\ 0 & \varepsilon \end{bmatrix}, \qquad \text{and} \qquad V^{-H} = \begin{bmatrix} 1 & 0 \\ -1/\varepsilon & 1/\varepsilon \end{bmatrix},$$

so that $y_1 = \widehat{x}_1 - \frac{1}{\varepsilon}\widehat{x}_2$ and $y_2 = \frac{1}{\varepsilon}\widehat{x}_2$ (both unnormalized). Hence,

$$\kappa(\alpha)^2 = \left(\frac{\|x_1\|\|y_1\|}{|x_1^H y_1|} \right)^2 = \frac{1 + \dfrac{1}{\varepsilon^2}}{\left(x_1^H x_1 - \dfrac{1}{\varepsilon}\widehat{x}_2^H x_1 \right)^2} = 1 + \frac{1}{\varepsilon^2},$$

$$\kappa(\beta)^2 = \left(\frac{\|x_2\|\|y_2\|}{|x_2^H y_2|} \right)^2 = \frac{(1+\varepsilon^2)\dfrac{1}{\varepsilon^2}}{\left(\dfrac{1}{\varepsilon}\widehat{x}_2^H x_1 + \widehat{x}_2^H \widehat{x}_2 \right)^2} = 1 + \frac{1}{\varepsilon^2}. \qquad \square$$

2.2. A new convergence analysis for two-dimensional ill-conditioning. For $A = \widehat{X} L \widehat{X}^H$ with $\widehat{X}$ unitary as in (2.2), let p be a polynomial of degree m. Then

$$p(A) = \widehat{X} \begin{bmatrix} p(L_1) & \\ & p(L_2) \end{bmatrix} \widehat{X}^H,$$

with

$$p(L_1) = \begin{bmatrix} 1 & 1 \\ & \varepsilon \end{bmatrix} p\left(\begin{bmatrix} \alpha & 0 \\ 0 & \beta \end{bmatrix} \right) \begin{bmatrix} 1 & 1 \\ & \varepsilon \end{bmatrix}^{-1} = \begin{bmatrix} p(\alpha) & \frac{p(\beta)-p(\alpha)}{\varepsilon} \\ 0 & p(\beta) \end{bmatrix}, \tag{2.4}$$

and $p(L_2) = \text{diag}(p(\lambda_3), \dots, p(\lambda_n))$.

TABLE 1

Values of GMRES *polynomial* p_m *at* $\beta = 4$ *and* $\alpha = 1.5$ *during the first* 10 *iterations. All other eigenvalues are contained in the interval* $[1, 2]$*, with* $\lambda_{10} = 1.1837$ *and* $\lambda_{20} = 1.3878$. $\lambda^{(m)}$ *is the largest in magnitude root of* p_m.

m	$\lvert\lambda^{(m)} - \beta\rvert$	$p_m(\beta)$	$p_m(\alpha)$	$\frac{\lvert p_m(\beta)-p_m(\alpha)\rvert}{\varepsilon}$	$p_m(\lambda_{10})$	$p_m(\lambda_{20})$
2	2.07e-02	8.4972e-03	8.4964e-03	8.5201e-03	1.55e-01	5.69e-02
3	3.09e-02	–2.1379e-02	–2.1377e-02	2.1380e-02	1.06e-02	–1.76e-02
4	3.51e-04	–4.0020e-04	–4.0016e-04	4.0044e-04	–2.13e-03	–3.16e-03
5	3.07e-04	5.8158e-04	5.8152e-04	5.8209e-04	–7.86e-04	1.95e-04
6	5.97e-06	1.8764e-05	1.8762e-05	1.7824e-05	–1.17e-04	1.07e-04
7	2.93e-06	–1.5262e-05	–1.5261e-05	1.3457e-05	–5.88e-06	4.52e-06
8	8.14e-08	–7.0406e-07	–7.0395e-07	1.1100e-06	1.93e-06	–2.57e-06
9	2.73e-08	3.9128e-07	3.9103e-07	2.5500e-06	5.98e-07	–3.55e-07
10	9.76e-10	2.3213e-08	2.3670e-08	4.5718e-06	8.23e-08	3.91e-08

For the GMRES residual norm we can thus exploit this structure to write

$$\|r_m\| = \min_{p\in\mathbb{P}_m^*} \|p(A)r_0\| = \min_{p\in\mathbb{P}_m^*} \|\widehat{X}p(L)\widehat{X}^H r_0\| = \min_{p\in\mathbb{P}_m^*} \|p(L)c_0\|, \tag{2.5}$$

where we have set $c_0 := \widehat{X}^H r_0$. We start by reporting on a simple experiment that motivates our analysis.

Example 2.3. Consider GMRES applied to $L = \text{blkdiag}(L_1, L_2)$ with $n = 50$, and a constant right-hand side with unit norm. We take $\alpha = 1.5$, $\beta = 4.0$, and $\lambda_3, \dots, \lambda_{50}$ uniformly distributed in $(1, 2)$, so that β is an outlier, while α is well inside the rest of the spectral interval.[2] Table 1 shows the values of the GMRES polynomial p_m at α, β and at a sample of other eigenvalues of L, namely $\lambda_{10}, \lambda_{20}$, during the first 10 iterations (at subsequent iterations the explicit computation of the polynomial was not fully reliable, as can be observed in the last two rows). The quantity $|p_m(\beta)-p_m(\alpha)|/\varepsilon$ is also reported, for $\varepsilon = 10^{-4}$, together with the distance[3] of the largest root of the GMRES polynomial from the outlying eigenvalue 4. The numbers in the table show that the GMRES polynomial takes approximately the same values at α and β, in a way such that $|p_m(\beta) - p_m(\alpha)|/\varepsilon$ stays at the level of the other polynomial values. This seems to suggest that the GMRES minimization is done so as to balance the polynomial magnitude at all nonzero entries of $p_m(L_1)$ and $p_m(L_2)$, in spite of the small ε. In other words, the magnitude of p_m at α and β is the same throughout the convergence history; we noticed this behavior for a large variety of distributions of α, β, both inside and outside the rest of the spectral interval.

We next build upon this argument to form such a "constrained" polynomial in an more explicit way. Clearly, from (2.5) we get $\|p(L)c_0\|^2 = \|p(L_1){c_0}^{(1)}\|^2 + \|p(L_2){c_0}^{(2)}\|^2$. We have

$$\|p(L_1)\| \le \max\{|p(\alpha)|, |p(\beta)|\} + \frac{|p(\beta) - p(\alpha)|}{\varepsilon}, \tag{2.6}$$

and therefore, recalling that $\alpha = \lambda_1, \beta = \lambda_2$, we have

$$\|r_m\| \le \min_{p\in\mathbb{P}_m^*} \left(\max_i |p(\lambda_i)| + \frac{|p(\beta) - p(\alpha)|}{\varepsilon} \right) \|c_0\|.$$

[2]Different distributions of α, β will be considered in later experiments, with similar behaviors.

[3]Interestingly, if the outlying eigenvalue $\lambda = 4$ belongs to the well-behaved group in L_2, its approximation by a root of the GMRES polynomial is significantly faster.

The upper bound aims at minimizing the quantity $\frac{|p(\beta)-p(\alpha)|}{\varepsilon}$, especially for small ε, while trying to be minimal at all the eigenvalues. This can also be appreciated by writing down $\|p(L_1)\|_F$. For this reason, we propose to bound the norm associated with the optimal residual polynomial by one that satisfies the additional constraint

$$p(\beta) = \frac{p(\beta)-p(\alpha)}{\varepsilon}, \tag{2.7}$$

so that the (1,2) entry of the rightmost matrix in (2.4) is forced to be the same as the (2,2) entry. Other choices could be considered; see Remark 2.6. The constraint (2.7) can be reformulated as

$$p(\alpha) = (1-\varepsilon)p(\beta) \quad \text{or, for } p(\beta) \neq 0, \quad \text{as} \quad \frac{p(\beta)-p(\alpha)}{p(\beta)} = \varepsilon; \tag{2.8}$$

the constraint can be interpreted as a request for $p(\alpha)$ and $p(\beta)$ to be as close as the value of ε, in a relative sense.

By asking $(p(\beta)-p(\alpha))/\varepsilon$ to assume a precise value, we are thus implicitly imposing conditions regarding the quotient $(p(\beta)-p(\alpha))/(\beta-\alpha)$, because

$$\frac{p(\beta)-p(\alpha)}{\varepsilon} = \frac{p(\beta)-p(\alpha)}{\beta-\alpha}\frac{\beta-\alpha}{\varepsilon}.$$

In the case when α and β are close to each other, we are implicitly imposing conditions on the first derivative of the minimal polynomial. We will return to this observation in section 3.

We are ready to state the main result of this section, which describes the effect of the new constraint in (2.7) on the GMRES residual bound.

THEOREM 2.4. *Let the diagonalizable matrix A be defined as in* (2.2)*, and let $c_0 := \widehat{X}^H r_0$. Then at every step $m \geq 2$ the* GMRES *residual norm satisfies*

$$\|r_m\| \leq \sqrt{3} \min_{\substack{p\in\mathbb{P}_m^* \\ p(\beta)=\frac{p(\beta)-p(\alpha)}{\varepsilon}}} \|p(\Lambda)c_0\|. \tag{2.9}$$

Proof. We have

$$\begin{aligned}\|r_m\|^2 &= \min_{p\in\mathbb{P}_m^*} \|p(A)r_0\|^2 = \min_{p\in\mathbb{P}_m^*} \left(\|p(L_1){c_0}^{(1)}\|^2 + \|p(L_2){c_0}^{(2)}\|^2\right) \\ &\leq \min_{\substack{p\in\mathbb{P}_m^* \\ p(\beta)=\frac{p(\beta)-p(\alpha)}{\varepsilon}}} \left(\|p(L_1){c_0}^{(1)}\|^2 + \|p(L_2){c_0}^{(2)}\|^2\right).\end{aligned}$$

With the constraint (2.7), the expression in (2.4) gives

$$\begin{aligned}\|p(L_1){c_0}^{(1)}\|^2 &= \left\|\begin{bmatrix} p(\alpha) & p(\beta) \\ & p(\beta)\end{bmatrix}{c_0}^{(1)}\right\|^2 = \left\|\begin{bmatrix} 1 & 1 \\ & 1\end{bmatrix}\begin{bmatrix} p(\alpha) & \\ & p(\beta)\end{bmatrix}{c_0}^{(1)}\right\|^2 \\ &\leq 3\left\|\begin{bmatrix} p(\alpha) & \\ & p(\beta)\end{bmatrix}{c_0}^{(1)}\right\|^2.\end{aligned} \tag{2.10}$$

The constant 3 is an upper bound for $\frac{3+\sqrt{5}}{2} \approx 2.6$, the squared norm of the 2×2

Jordan matrix $[1,1;0,1]$. Therefore,

$$\begin{aligned}\|r_m\|^2 &\le \min_{\substack{p\in\mathbb{P}_m^*\\ p(\beta)=\frac{p(\beta)-p(\alpha)}{\varepsilon}}} 3\left(\left\|\begin{bmatrix}p(\alpha) & \\ & p(\beta)\end{bmatrix} {c_0}^{(1)}\right\|^2 + \|p(L_2){c_0}^{(2)}\|^2\right)\\ &= \min_{\substack{p\in\mathbb{P}_m^*\\ p(\beta)=\frac{p(\beta)-p(\alpha)}{\varepsilon}}} 3\|p(\Lambda)c_0\|^2,\end{aligned}$$

from which the result follows. ◻

Several remarks are in order. First, we note that the bound in (2.9) is surprisingly clean, involving nothing but the eigenvalues of A and the initial residual. No condition number of the whole eigenvector matrix (or parts of it) appears as a factor; the parameter ε associated with the ill-conditioning only appears in the constraint, in a less harmful manner. Second, the bound does not depend on how close α and β are. In other words, it can be descriptive irrespective of the distribution of the eigenvalues. Third, the bound in Theorem 2.4 can be further estimated as

$$\|r_m\| \le \sqrt{3} \min_{\substack{p\in\mathbb{P}_m^*\\ p(\beta)=\frac{p(\beta)-p(\alpha)}{\varepsilon}}} \max_{i=1,\ldots,n} |p(\lambda_i)|\|r_0\|,$$

which leads to a constrained min-max polynomial problem.

Remark 2.5. Using the relation (2.8), we can write

$$\|r_m\| \le \sqrt{3} \min_{\substack{p\in\mathbb{P}_m^*\\ p(\alpha)=(1-\varepsilon)p(\beta)}} \|p(\breve{\Lambda})\breve{c}_0\|,$$

where $\breve{\Lambda} = \mathrm{diag}(\beta,\beta,\lambda_3,\ldots,\lambda_n)$ and $\breve{c}_0 = ((1-\varepsilon)c_{0,1}, c_{0,2},\ldots,c_{0,n})^T$. Indeed, thanks to (2.8) we have

$$\begin{aligned}\|p(\Lambda)c_0\|^2 &= \sum_{i=1}^n p(\lambda_i)^2 c_{0,i}^2 = p(\alpha)^2 c_{0,1}^2 + p(\beta)^2 c_{0,2}^2 + \sum_{i=3}^n p(\lambda_i)^2 c_{0,i}^2\\ &= p(\beta)^2(1-\varepsilon)^2 c_{0,1}^2 + p(\beta)^2 c_{0,2}^2 + \sum_{i=3}^n p(\lambda_i)^2 c_{0,i}^2 = \|p(\breve{\Lambda})\breve{c}_0\|^2.\end{aligned}$$

Remark 2.6. The constraint that the ratio $(p(\beta)-p(\alpha))/\varepsilon$ be equal to $p(\beta)$ is somewhat arbitrary, though it makes the final bound of Theorem 2.4 particularly clean. Among others, the choices

$$\frac{p(\beta)-p(\alpha)}{\varepsilon} = p(\alpha) \quad \text{and} \quad \frac{p(\beta)-p(\alpha)}{\varepsilon} = \frac{p(\beta)+p(\alpha)}{2}$$

achieve a similar goal and could also be considered. The first case was commented on in [24]. In the second case we would have

$$p(L_1) = \begin{bmatrix}1 & \frac12\\ 0 & 1\end{bmatrix}\begin{bmatrix}p(\alpha) & 0\\ 0 & p(\beta)\end{bmatrix}\begin{bmatrix}1 & \frac12\\ 0 & 1\end{bmatrix}.$$

The right upper triangular matrix would then interfere with the residual vector in the derivation (2.10).

2.3. Numerical experiments. In this first set of experiments we illustrate the quality of the new bound in (2.9) on eigenvalue pairs, for different choices of their location. The constrained optimization problem that leads to the new bound was numerically solved with the MATLAB built-in function `fsolve`: the reported results were obtained through both the Trust-Region Dogleg and the Levenberg–Marquardt algorithms (depending on which behaved best in terms of convergence and stability) [21]. We refer the reader to the appendix and to [24] for more details.

The polynomial giving the numerical solution of this problem is denoted by p_{con}. Without loss of generality, for our purposes all examples consider small size coefficient matrices, which make it possible to compute all quantities of interest and illustrate our theoretical results.

Example 2.7. We present four variants of the same spectrum with initial distribution of integer values between 1 and 50. We ascribe the ill-conditioning to the pairs $(\alpha, \beta) = (49, 50)$, $(\alpha, \beta) = (1, 50)$, $(\alpha, \beta) = (30.5, 30.5001)$, and $(\alpha, \beta) = (1, 2)$ in sequence; in this third case, α and β replace the eigenvalues 1 and 2. In all considered cases, α and β are not outliers with respect to the considered spectral interval. The stopping tolerance for the linear and nonlinear solvers was set to 10^{-8}, while $\varepsilon = 10^{-4}$.

In all cases except the third, the two ill-conditioned eigenvalues are chosen to be relatively distant from each other. In particular, in the first case α and β are on the right end of the spectrum, in the last case on the left end, and in the second case they delimit the remaining eigenvalues. Tables 2–5 report the number of iterations k, the number of optimization iterations, and then the norm of the constrained polynomial, the GMRES residual norm, and the relative difference between these last two quantities. All tables show that the optimal polynomial associated with the constrained minimization problem of Theorem 2.4 gives a bound that strictly follows the GMRES convergence curve, with high relative accuracy. The small distance between α and β of the third case does not seem to affect the quality of the results. In most cases, the constrained problem is solved in a very small number of iterations, showing that the starting guess, corresponding to the current GMRES polynomial, is very close to the sought-after solution, within the given tolerance. As an extreme case, in the third table the GMRES polynomial already satisfied the tolerance, so that the nonlinear solver needed zero iterations.

3. Similarities and dissimilarities with the 2×2 Jordan case. In this section we explore the closeness of L_1 to a Jordan block. It turns out that for ε small, similarities occur even when α and β are not close to each other.

When A is not diagonalizable, a relation similar to (1.1), involving the Jordan form of A, can be derived. We report here the result, which is along the same line as that for QMR described in [8]; for an explicit proof in the case of GMRES, we refer the reader to [24] and [16, section 5.7.2].

THEOREM 3.1. *Let A be a nonsingular $n\times n$ matrix, with eigenvalues $\lambda_1, \ldots, \lambda_r$ of algebraic multiplicity $\mu_1, \ldots, \mu_r$, respectively, and Jordan form $A = XJX^{-1}$. Denote by $J(\lambda_k)$ the largest Jordan block corresponding to the eigenvalue λ_k; let $\ell_k \le \mu_k$ be*

TABLE 2
Example 2.7, case 1. Eigenvalues uniformly distributed in $[1, 50]$, $\alpha = 50$, $\beta = 49$.

k	$iter_{fsolve}$	$\|p_{con}(L)r_0\|$	$\|r_k\|$	$\frac{\|p_{con}(L)r_0\| - \|r_k\|}{\|r_k\|}$
5	1	1.45e-01	1.45e-01	6.50e-15
10	2	4.49e-02	4.49e-02	5.10e-15
15	1	1.08e-02	1.08e-02	3.83e-13
20	1	1.57e-03	1.57e-03	7.88e-15
25	1	1.26e-04	1.26e-04	4.31e-15
30	1	5.12e-06	5.12e-06	2.85e-12
35	1	9.36e-08	9.36e-08	1.92e-12

TABLE 3
Example 2.7, case 2. Eigenvalues uniformly distributed in $[1, 50]$, $\alpha = 1$, $\beta = 50$.

k	$iter_{fsolve}$	$\|p_{con}(L)r_0\|$	$\|r_k\|$	$\frac{\|p_{con}(L)r_0\| - \|r_k\|}{\|r_k\|}$
5	1	1.91e-01	1.91e-01	4.05e-11
10	3	4.31e-02	4.31e-02	1.05e-10
15	2	1.09e-02	1.09e-02	1.51e-10
20	1	1.57e-03	1.57e-03	1.77e-10
25	1	1.26e-04	1.26e-04	2.00e-10
30	1	5.12e-06	5.12e-06	2.23e-10
35	1	9.36e-08	9.36e-08	2.21e-10

TABLE 4
Example 2.7, case 3. $\alpha = 30.5$, $\beta = 30.5001$, *other eigenvalues uniformly distributed in* $[3, 50]$.

k	$iter_{fsolve}$	$\|p_{con}(L)r_0\|$	$\|r_k\|$	$\frac{\|p_{con}(L)r_0\| - \|r_k\|}{\|r_k\|}$
5	0	6.93e-02	6.93e-02	–3.43e-14
10	0	6.71e-03	6.71e-03	2.06e-14
15	0	5.03e-04	5.03e-04	–6.67e-15
20	0	2.63e-05	2.63e-05	5.90e-14
25	0	8.58e-07	8.58e-07	3.20e-15
30	0	1.52e-08	1.52e-08	–1.89e-13

TABLE 5
Example 2.7, case 4. $\alpha = 1$, $\beta = 2$, *other eigenvalues uniformly distributed in* $[3, 50]$.

k	$iter_{fsolve}$	$\|p_{con}(L)r_0\|$	$\|r_k\|$	$\frac{\|p_{con}(L)r_0\| - \|r_k\|}{\|r_k\|}$
5	17	1.45e-01	1.45e-01	4.20e-15
10	2	4.48e-02	4.48e-02	-2.31e-15
15	2	1.07e-02	1.07e-02	-1.89e-14
20	27	1.56e-03	1.56e-03	5.94e-15
25	22	1.25e-04	1.25e-04	-4.31e-15
30	48	5.12e-06	5.12e-06	-3.30e-16
35	9	9.35e-08	9.35e-08	1.71e-12

its order. Then it holds that

$$\frac{\|r_m\|}{\|r_0\|} \le \kappa(X) \min_{p \in \mathbb{P}_m^*} \max_{k=1,\dots,r} \|p(J(\lambda_k))\| \tag{3.1}$$

$$\le \kappa(X) \min_{p \in \mathbb{P}_m^*} \max_{k=1,\dots,r} \left(\sum_{j=0}^{\ell_k - 1} \frac{1}{j!} \left| p^{(j)}(\lambda_k) \right| \right). \tag{3.2}$$

While the theory regarding nondiagonalizable matrices involves not only the polynomial p but also its derivatives (see (3.2)), no derivatives appear when A is diagonalizable. However, if indeed A is a perturbation of a nondiagonalizable matrix, then disregarding derivatives may be misleading. In fact, we expect that the presence of a derivative, or at least a difference ratio, would provide a more descriptive bound. The new bound of Theorem 2.4 follows up on this argument by including a related constraint. In this section we explore the closeness of the diagonalizable and nondiagonalizable problems in terms of the GMRES residual polynomial. Let us recall the definition of L_1,

$$L_1 = \begin{bmatrix} \alpha & \frac{\beta-\alpha}{\varepsilon} \\ & \beta \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 0 & \varepsilon \end{bmatrix} \begin{bmatrix} \alpha & 0 \\ 0 & \beta \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & \varepsilon \end{bmatrix}^{-1} =: V \begin{bmatrix} \alpha & 0 \\ 0 & \beta \end{bmatrix} V^{-1}, \tag{3.3}$$

and let us introduce the nondiagonalizable matrix

$$\begin{aligned} L_{1,J} &= \begin{bmatrix} \alpha & \frac{\beta-\alpha}{\varepsilon} \\ \frac{-\varepsilon(\beta-\alpha)}{4} & \beta \end{bmatrix} \\ &= \begin{bmatrix} 1 & 1 \\ \frac{\varepsilon}{2} & \frac{\varepsilon}{\beta-\alpha}\left(1+\frac{\beta-\alpha}{2}\right) \end{bmatrix} \begin{bmatrix} \frac{\alpha+\beta}{2} & 1 \\ 0 & \frac{\alpha+\beta}{2} \end{bmatrix} \begin{bmatrix} 1 & 1 \\ \frac{\varepsilon}{2} & \frac{\varepsilon}{\beta-\alpha}\left(1+\frac{\beta-\alpha}{2}\right) \end{bmatrix}^{-1} \\ &=: V_J \begin{bmatrix} \frac{\alpha+\beta}{2} & 1 \\ 0 & \frac{\alpha+\beta}{2} \end{bmatrix} V_J^{-1} \end{aligned} \tag{3.4}$$

having the single eigenvalue $\frac{\alpha+\beta}{2}$ of index 2 (see [5, Example 4.2.2]). Note that the eigenvalue multiplicity of $L_{1,J}$ does not depend on α and β being close. For small ε, and also—but not necessarily—for α and β close to each other, the 2×2 matrix L_1 can be read as the perturbation of $L_{1,J}$. The absolute and relative differences between L_1 and $L_{1,J}$ are given by

$$\|L_1 - L_{1,J}\| = \frac{\varepsilon|\beta-\alpha|}{4}, \qquad \frac{\|L_1 - L_{1,J}\|}{\|L_{1,J}\|} \le \frac{\varepsilon^2}{2\sqrt{2}},$$

where we have used $\|L_{1,J}\| \ge \frac{1}{\sqrt{2}}\|L_{1,J}\|_F \ge \frac{|\beta-\alpha|}{\varepsilon\sqrt{2}}$. Therefore, whenever $|\beta-\alpha|$ is small, that is, the eigenvalues are close to each other, L_1 is close to the nondiagonalizable matrix $L_{1,J}$ in an absolute sense; whenever ε is small, L_1 is close to $L_{1,J}$ in both an absolute and a relative sense. This last observation highlights the fact that for L_1 and $L_{1,J}$ to be close it is unnecessary for α and β to be the perturbation of a single eigenvalue; even when α and β are far apart, L_1 may always be related to the nondiagonalizable matrix $L_{1,J}$, whose multiple eigenvalue is $\xi = (\alpha+\beta)/2$. For $\alpha \approx \beta$ this spectral connection is expected (see, e.g., the discussion in [26]), but it is less so when α and β are clearly separate. In summary, under the stated hypotheses, for small ε the matrix A is close to a nondiagonalizable matrix with a multiple eigenvalue at $(\alpha+\beta)/2$, irrespective of how close α and β are.

These considerations motivate further investigation aimed at comparing the behavior of the GMRES residual when applied to either $\text{blkdiag}(L_1, L_2)x = c_0$ or $\text{blkdiag}(L_{1,J}, L_2)x = c_0$. For analogy with A, we set $A_J := \text{blkdiag}(L_{1,J}, L_2)$. We refer the reader to, e.g., [25] for a recent discussion on the GMRES convergence for perturbed matrices. Here we only aim at analyzing the connection between our ill-conditioning model and the related Jordan block in the GMRES context.

To study the convergence behavior of GMRES, first we link more closely $p(L_1)$ and

$p(L_{1,J})$ for a polynomial p. We readily notice that

$$\|p(L_1)\| \le \|p(L_1)\|_F = \sqrt{|p(\alpha)|^2 + |p(\beta)|^2 + \left|\frac{p(\beta)-p(\alpha)}{\varepsilon}\right|^2}, \tag{3.5}$$

where the rewriting

$$\left|\frac{p(\beta)-p(\alpha)}{\varepsilon}\right|^2 = \left|\frac{p(\beta)-p(\alpha)}{\beta-\alpha}\right|^2 \left(\frac{|\beta-\alpha|}{\varepsilon}\right)^2$$

highlights the roles of the derivative of p and of the ratio $|\beta-\alpha|/\varepsilon$ in the particular case when $\beta-\alpha \to 0$. These will be made clearer in what follows.

Let $\xi = \frac{\alpha+\beta}{2}$. Then we have

$$\begin{aligned} p(L_{1,J}) &= V_J p\left(\begin{bmatrix} \xi & 1 \\ 0 & \xi \end{bmatrix}\right) V_J^{-1} = V_J \left(p(\xi)\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + p'(\xi)\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}\right) V_J^{-1} \\ &= p\left(\xi\right)\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + p'\left(\xi\right) V_J \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} V_J^{-1} \\ &= p(\xi)\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + p'(\xi)\frac{\beta-\alpha}{2}\begin{bmatrix} -1 & \frac{2}{\varepsilon} \\ -\frac{\varepsilon}{2} & 1 \end{bmatrix}. \qquad (3.6) \end{aligned}$$

Let us focus on the case when the distance between the two eigenvalues is small, i.e., $|\beta-\alpha| \ll 1$. To proceed, we need some Taylor expansions around ξ,

$$p(\alpha) = p\left(\xi - \frac{\beta-\alpha}{2}\right) = p(\xi) - p'(\xi)\frac{\beta-\alpha}{2} + \mathcal{O}(|\beta-\alpha|^2), \tag{3.7}$$

$$p(\beta) = p\left(\xi + \frac{\beta-\alpha}{2}\right) = p(\xi) + p'(\xi)\frac{\beta-\alpha}{2} + \mathcal{O}(|\beta-\alpha|^2), \tag{3.8}$$

so that

$$p(\beta) - p(\alpha) = p'(\xi)(\beta-\alpha) + \mathcal{O}(|\beta-\alpha|^2). \tag{3.9}$$

LEMMA 3.2. *For $|\beta-\alpha| \to 0$ it holds that*

$$\|p(L_1)\| \le |p(\xi)| + |p'(\xi)|\frac{|\beta-\alpha|}{2\varepsilon}\sqrt{2\varepsilon^2+4} + \mathcal{O}(|\beta-\alpha|^2) \tag{3.10}$$

and

$$\|p(L_{1,J})\| \le |p(\xi)| + |p'(\xi)|\frac{|\beta-\alpha|}{2\varepsilon}\left(2 + \frac{\varepsilon^2}{2}\right). \tag{3.11}$$

Proof. Substituting (3.7), (3.8), and (3.9) in (2.4), we can write

$$p(L_1) = p(\xi)I_2 + p'(\xi)\frac{\beta-\alpha}{2}\begin{bmatrix} -1 & 2/\varepsilon \\ & 1 \end{bmatrix} + \mathcal{O}(|\beta-\alpha|^2).$$

Therefore, collecting ε^{-1}, we have

$$\|p(L_1)\| \le |p(\xi)| + |p'(\xi)|\frac{|\beta-\alpha|}{2\varepsilon}\left\|\begin{bmatrix} -\varepsilon & 2 \\ & \varepsilon \end{bmatrix}\right\| + \mathcal{O}(|\beta-\alpha|^2).$$

The norm of the upper triangular matrix is bounded by its Frobenius norm, $\sqrt{2\varepsilon^2+4}$, from which the first bound follows.

For the second bound we use (3.6) to write

$$\|p(L_{1,J})\| \le |p(\xi)| + |p'(\xi)|\frac{|\beta-\alpha|}{2}\left\|\begin{bmatrix}-1 & 2/\varepsilon\\ -\varepsilon/2 & 1\end{bmatrix}\right\|.$$

Once again we bound the norm of the matrix in the right-hand side with its Frobenius norm, namely $(\frac{2}{\epsilon}+\frac{\epsilon}{2})$, thus completing the proof. □

The following results hold for the matrix polynomials $p(L_1)$, $p(L_{1,J})$.

PROPOSITION 3.3. *Consider L_1 and $L_{1,J}$ as defined in* (3.3) *and* (3.4)*, respectively. For fixed $\varepsilon > 0$ and for any polynomial p it holds that*

$$p(L_1) = p(L_{1,J}) + p'(\xi)\begin{bmatrix}0 & 0\\ \varepsilon\frac{\beta-\alpha}{4} & 0\end{bmatrix} + \mathcal{O}(|\beta-\alpha|^2)\begin{bmatrix}1 & 1\\ 0 & 1\end{bmatrix}$$

so that for $|\beta-\alpha|\to 0$,

$$\|p(L_1) - p(L_{1,J})\| = |p'(\xi)|\frac{|\beta-\alpha|}{4}\varepsilon + \mathcal{O}(|\beta-\alpha|^2). \tag{3.12}$$

Proof. Using (2.4), (3.6) and then (3.7), (3.8), and (3.9), we obtain

$$\begin{aligned} p(L_1) - p(L_{1,J}) &= \begin{bmatrix}p(\alpha) & \frac{p(\beta)-p(\alpha)}{\varepsilon}\\ 0 & p(\beta)\end{bmatrix} - p(\xi)\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix} - p'(\xi)\frac{\beta-\alpha}{2}\begin{bmatrix}-1 & \frac{2}{\varepsilon}\\ -\frac{\varepsilon}{2} & 1\end{bmatrix}\\ &= p'(\xi)\begin{bmatrix}-\frac{\beta-\alpha}{2} & \frac{\beta-\alpha}{\varepsilon}\\ 0 & \frac{\beta-\alpha}{2}\end{bmatrix} - p'(\xi)\frac{\beta-\alpha}{2}\begin{bmatrix}-1 & \frac{2}{\varepsilon}\\ -\frac{\varepsilon}{2} & 1\end{bmatrix} + \mathcal{O}(|\beta-\alpha|^2)\begin{bmatrix}1 & 1\\ 0 & 1\end{bmatrix}\\ &= p'(\xi)\begin{bmatrix}0 & 0\\ \varepsilon\frac{\beta-\alpha}{4} & 0\end{bmatrix} + \mathcal{O}(|\beta-\alpha|^2)\begin{bmatrix}1 & 1\\ 0 & 1\end{bmatrix},\end{aligned}$$

and the result follows. □

Proposition 3.3 shows that for any polynomial p such that $|p'(\xi)|$ is not excessively large, the value of $p(L_1)$ is close to that of $p(L_{1,J})$ when the distance between α and β (eigenvalues of L_1) is small. In fact, the proximity is even stronger for small ε; in this case, indeed, a very small $\varepsilon|\beta-\alpha|$ can control a possibly large value of the derivative of p at ξ. As a consequence, when the eigenvalues α and β are close to each other and ε is also possibly small, the GMRES residual history of $Ax = b$ closely follows that of $A_J x = b$ (clearly, for $|\beta-\alpha| \gg 0$, the behavior may differ). Note that this behavior is different from the case $\varepsilon \gg 0$—so that $|p'(\xi)|\frac{|\beta-\alpha|}{4}\varepsilon$ may not be sufficiently small—in which case close eigenvalues do not necessarily imply close convergence behavior [16, sections 5.6.4 and 5.6.5]. The considerations above are summarized in the following proposition.

PROPOSITION 3.4. *Denote with r_m and $r_{m,J}$ the mth residuals of* GMRES *applied to $Ax = b$ and $A_J x = b$, respectively, with $r_0 = b - Ax_0 = [r_0^{(1)}; r_0^{(2)}]$ partitioned accordingly with L_1, L_2. Let $p_m(z)$ and $p_{m,J}(z)$ be the corresponding residual polynomials. Finally, let $\xi = \frac{\alpha+\beta}{2}$. Then for $|\beta-\alpha|\to 0$,*

$$\Big|\|r_m\| - \|r_{m,J}\|\Big| \le \max\left\{|p_m'(\xi)|\,,\,|p_{m,J}'(\xi)|\right\}\frac{|\beta-\alpha|}{4}\varepsilon\|r_0^{(1)}\| + \mathcal{O}(|\beta-\alpha|^2). \tag{3.13}$$

Proof.

$$\begin{aligned}
\|r_m\| &= \min_{p\in\mathbb{P}_m^*} \|p(A)r_0\| \le \|p_{m,J}(A)r_0\| \\
&\le \|p_{m,J}(A_J)r_0\| + \|p_{m,J}(A)r_0 - p_{m,J}(A_J)r_0\| \\
&= \|r_{m,J}\| + \|(p_{m,J}(A) - p_{m,J}(A_J))r_0\| \\
&= \|r_{m,J}\| + \left\| \begin{bmatrix} p_{m,J}(L_1) - p_{m,J}(L_{1,J}) & 0 \\ 0 & p_{m,J}(L_2) - p_{m,J}(L_2) \end{bmatrix} c_0 \right\| \\
&= \|r_{m,J}\| + \left\| \begin{bmatrix} p_{m,J}(L_1) - p_{m,J}(L_{1,J}) & 0 \\ 0 & 0 \end{bmatrix} c_0 \right\| \\
&= \|r_{m,J}\| + \left\| (p_{m,J}(L_1) - p_{m,J}(L_{1,J}))\, {c_0}^{(1)} \right\|.
\end{aligned}$$

Thus, using (3.12), for $|\beta-\alpha| \to 0$ we obtain

$$\|r_m\| \le \|r_{m,J}\| + \left|p'_{m,J}(\xi)\right| \frac{|\beta-\alpha|}{4}\varepsilon\|{c_0}^{(1)}\| + \mathcal{O}(|\beta-\alpha|^2).$$

In the same way, we can write

$$\|r_{m,J}\| \le \|r_m\| + |p'_m(\xi)| \frac{|\beta-\alpha|}{4}\varepsilon\|{c_0}^{(1)}\| + \mathcal{O}(|\beta-\alpha|^2).$$

Combining the last two inequalities, we obtain the result. ∎

In the next example we illustrate the relation (3.4) for α and β close to each other.

Example 3.5. We report on the behavior of GMRES on A and A_J when α, β are close to each other, so that they can be viewed as a perturbation of $\xi = (\alpha+\beta)/2$. We consider $\alpha = 1, \beta = \alpha + 10^{-2}$, while the other eigenvalues are $3, 4, \dots, 50$. Here $\varepsilon = 10^{-3}(\beta-\alpha)$. The left plot of Figure 1 shows the GMRES convergence curves (blue "-×-" and large black "· · + · ·" symbols), together with the convergence history obtained with p_{con}, the constrained polynomial ("-∘-" symbol). We can see that the three curves visually coincide up to convergence. To complete the picture, we also report the GMRES convergence history for the following two additional matrices, recalling that $\widehat{X}$ is unitary:

A_D: normal matrix obtained as $A_D = \widehat{X}\mathrm{diag}(\alpha, \beta, \lambda_3, \dots, \lambda_n)\widehat{X}^*$ (thick green "· · + · ·" symbol);

A_{D_ξ}: normal matrix obtained as $A_{D_\xi} = \widehat{X}\mathrm{diag}(\xi, \xi, \lambda_3, \dots, \lambda_n)\widehat{X}^*$ (magenta "· · × · ·" symbol).

Note that although both A_D and A_{D_ξ} are in fact real symmetric in this simple illustrative example, similar results can be obtained for complex spectra (see, e.g., [24]). Thus, we prefer to keep the discussion as general as possible and keep the term "normal" throughout.

The behavior of GMRES significantly differs at the early convergence stage when these two normal matrices are considered, illustrating quite clearly where the ill-conditioning of the eigenvector pair delays convergence on the system with A. The GMRES polynomial needs to also be smooth at α and β when eigenvector ill-conditioning is present (see, e.g., the discussion preceding relation (3.10) and Lemma 3.2), and this is well captured by the constrained polynomial. It is also interesting to observe that at a residual norm slightly below 10^{-3}, the convergence curves for A_D and A_{D_ξ} split,

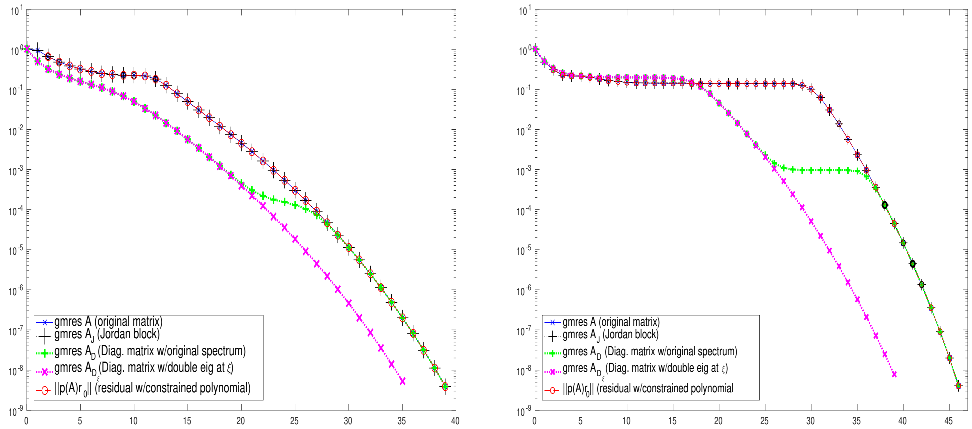

FIG. 1. *Behavior of* GMRES *on A and A_J with $\lambda_j \in \{3,\dots,50\}$, $j \geq 3$. Left: $\varepsilon = 10^{-3}(\beta-\alpha)$, $\alpha = 1$, $\beta = \alpha + 10^{-2}$. Right: $\varepsilon = 10^{-1}(\beta-\alpha)$, $\alpha = 0.01$, $\beta = \alpha + 10^{-4}$. Color is available online only.*

as if it is only at that point the method realizes the two eigenvalues α and β are actually different from ξ. The discrepancies in the behavior for A_D and A_{D_ξ} are in agreement with the comments in [16, sections 5.6.4 and 5.6.5] for the symmetric case.

The right plot of Figure 1 shows a similar, though more pronounced, behavior for the case when $\alpha = 0.01$, $\beta = \alpha + 10^{-4}$, and $\varepsilon = 10^{-1}(\beta-\alpha)$.

4. An analysis for close invariant subspaces. We first construct a matrix A having a block of ill-conditioned eigenvectors. Let us consider the *unitary* matrix $\widehat{X} = [\widehat{X}_1, \widehat{X}_2, \widehat{X}_3]$, $\widehat{X}_2 \in \mathbb{C}^{n\times \ell_2}$, $\widehat{X}_3 \in \mathbb{C}^{n\times \ell_3}$, $\widehat{X}_1 \in \mathbb{C}^{n\times(n-\ell_2-\ell_3)}$, and the eigenvector matrix

$$X = [\widehat{X}_1, \widehat{X}_2, X_3], \tag{4.1}$$

with

$$X_3 := \widehat{X}_2 R_0 + \varepsilon \widehat{X}_3, \tag{4.2}$$

for some full rank rectangular matrix R_0 of conforming dimension, such that $\|R_0\| \approx 1$. For small $\varepsilon > 0$ the columns of $\widehat{X}_2$ and X_3 span closely related subspaces; note that each column of X has approximately unit norm. Then

$$X = \widehat{X} \begin{bmatrix} I & & \\ & I & R_0 \\ & & \varepsilon I \end{bmatrix} =: \widehat{X}\widehat{R},$$

and for our choice of X_3, the matrix X is nonsingular. We note in passing that in the matrix X, the first block $\widehat{X}_1$ is still orthogonal to $\widehat{X}_2$ and to the newly formed X_3. We define A through its eigendecomposition as $A = X\Lambda X^{-1}$ with the block partitioning $\Lambda = \mathrm{blkdiag}(\Lambda_1, \Lambda_2, \Lambda_3)$, conforming to the blocking of X. We have

$$A = X\Lambda X^{-1} = \widehat{X}\widehat{R}\Lambda\widehat{R}^{-1}\widehat{X}^H \tag{4.3}$$

$$= \widehat{X} \begin{bmatrix} I & & \\ & I & R_0 \\ & & \varepsilon I \end{bmatrix} \begin{bmatrix} \Lambda_1 & & \\ & \Lambda_2 & \\ & & \Lambda_3 \end{bmatrix} \begin{bmatrix} I & & \\ & I & -\varepsilon^{-1}R_0 \\ & & \varepsilon^{-1} I \end{bmatrix} \widehat{X}^H. \tag{4.4}$$

Moreover,

$$p(A) = Xp(\Lambda)X^{-1} = \widehat{X}\begin{bmatrix} p(\Lambda_1) & & \\ & p(\Lambda_2) & \frac{1}{\varepsilon}(-p(\Lambda_2)R_0 + R_0p(\Lambda_3)) \\ & & p(\Lambda_3)\end{bmatrix}\widehat{X}^H. \tag{4.5}$$

We thus impose the matrix constraint

$$\frac{1}{\varepsilon}\left(R_0p(\Lambda_3) - p(\Lambda_2)R_0\right) = R_0p(\Lambda_3) \tag{4.6}$$

or, equivalently,

$$p(\Lambda_2)R_0 = R_0p(\Lambda_3)(1-\varepsilon), \quad R_0 \in \mathbb{C}^{\ell_2\times\ell_3}. \tag{4.7}$$

Therefore, if $\ell_2 \geq \ell_3$, the constraint (4.6) amounts to requiring that the diagonal values of $p(\Lambda_3)(1-\varepsilon)$ coincide with some of those of $p(\Lambda_2)$ (the columns of R_0 span an invariant subspace of $p(\Lambda_2)$). If $\ell_3 \geq \ell_2$, the same statement holds but with the roles reversed.

The next theorem extends Theorem 2.4 to the case of an ill-conditioned eigenspace.

THEOREM 4.1. *Let $A = X\Lambda X^{-1}$, and assume that X can be written as in* (4.1), *so that for $\varepsilon > 0$ there exists a full rank matrix R_0 such that* (4.2) *holds. Then after m iterations the* GMRES *residual satisfies*

$$\|r_m\| \leq \gamma \min_{\substack{p\in\mathbb{P}_m^* \\ p(\Lambda_2)R_0 = R_0p(\Lambda_3)(1-\varepsilon)}} \|p(\Lambda)c_0\|, \tag{4.8}$$

where $\gamma \leq 1 + \|R_0\|$.

We note that in general m needs to be large enough so that the constraint can be imposed; this is obtained for $m \geq 1 + \ell_3$ if $\ell_2 \geq \ell_3$. However, the constraint may be satisfied for smaller values of m.

Proof. Following the proof of Theorem 2.4, by using (4.5) we obtain

$$\begin{aligned}\|r_m\|^2 = \min_{p\in\mathbb{P}_m^*}\|p(A)r_0\|^2 &= \min_{p\in\mathbb{P}_m^*}\left\|\begin{bmatrix} p(\Lambda_1) & & \\ & p(\Lambda_2) & \frac{R_0p(\Lambda_3)-p(\Lambda_2)R_0}{\varepsilon} \\ & & p(\Lambda_3)\end{bmatrix}c_0\right\|^2 \\ &\leq \min_{\substack{p\in\mathbb{P}_m^* \\ R_0p(\Lambda_3) = \frac{R_0p(\Lambda_3)-p(\Lambda_2)R_0}{\varepsilon}}}\left\|\begin{bmatrix} p(\Lambda_1) & & \\ & p(\Lambda_2) & R_0p(\Lambda_3) \\ & & p(\Lambda_3)\end{bmatrix}c_0\right\|^2,\end{aligned}$$

where (4.6) was used. For the lower triangular block we have

$$\begin{bmatrix} p(\Lambda_2) & R_0p(\Lambda_3) \\ & p(\Lambda_3)\end{bmatrix} = \begin{bmatrix} I & R_0 \\ & I\end{bmatrix}\begin{bmatrix} p(\Lambda_2) & \\ & p(\Lambda_3)\end{bmatrix}, \tag{4.9}$$

and therefore,

$$\|r_m\|^2 \leq \min_{\substack{p\in\mathbb{P}_m^* \\ p(\Lambda_2)R_0 = R_0p(\Lambda_3)(1-\varepsilon)}}\left\|\begin{bmatrix} I & & \\ & I & R_0 \\ & & I\end{bmatrix}\begin{bmatrix} p(\Lambda_1) & & \\ & p(\Lambda_2) & \\ & & p(\Lambda_3)\end{bmatrix}c_0\right\|^2$$

and for γ equal to the norm of the block matrix containing R_0, we finally find

$$\|r_m\| \leq \gamma \min_{\substack{p\in\mathbb{P}_m^* \\ p(\Lambda_2)R_0=R_0p(\Lambda_3)(1-\varepsilon)}} \|p(\Lambda)c_0\| . \qquad \square$$

The parameter γ has moderate magnitude by construction; if R_0 has orthonormal columns, then $\gamma = \sqrt{(3+\sqrt{5})/2}$.

Remark 4.2. The bound of Theorem 4.1 can be further estimated as

$$\|r_m\| \leq \gamma \min_{\substack{p\in\mathbb{P}_m^* \\ p(\Lambda_2)R_0=R_0p(\Lambda_3)(1-\varepsilon)}} \max_{i=1,\ldots,n} |p(\lambda_i)|\|r_0\|. \tag{4.10}$$

Remark 4.3. If R_0 is square, then the bound simplifies, as the constraint becomes $p(\Lambda_2) = p(\Lambda_3)(1-\varepsilon)$ for some reordering of the eigenvalues, so that we obtain, for instance,

$$\|r_m\| \leq \gamma \min_{\substack{p\in\mathbb{P}_m^* \\ p(\Lambda_2)=p(\Lambda_3)(1-\varepsilon)}} \max_{i=1,\ldots,n} |p(\lambda_i)|\|r_0\|.$$

This means that the polynomial at each eigenvalue of Λ_2 is assumed to take values that are a slight perturbation of the values taken at Λ_3. As a special case, if each column of X_3 is almost collinear to a different eigenvector in $\widehat{X}_2$, then $R_0 = I$ and the bound simplifies. This latter situation is the precise generalization of the two-dimensional ill-conditioning analyzed in section 2.

Example 4.4. We consider $n = 50$ randomly distributed eigenvalues in the open box $(0, 10^{-2})\times(0, 10^{-2}) \subset \mathbb{C}$. We take as elements of Λ_2 the first 10 of them (unsorted) and as Λ_3 the next 10; the matrix R_0 in (4.2) is the identity matrix of size 10; being square, it only enters the constrained problem computation into the definition of γ, which for this problem had a value of approximately 1.6. In this case $\varepsilon = 10^{-4}$. The matrix A was then constructed according to (4.3). Results in the left plot of Figure 2 essentially show what was already observed for a two-dimensional ill-conditioning problem, although now the bound of Theorem 4.1 is not as sharp. Nonetheless, the residual norm behavior is fully captured. For completeness we also report the convergence history of the normal problem obtained by dropping the matrix $\widehat{R}$ in the definition of A, so as to eliminate the ill-conditioning of the eigenvector matrix. It is interesting to observe that the initial 10-iteration stagnation matches the number of constraints to be imposed on the polynomial to comply with the ill-conditioning of the eigenbasis.

Example 4.5. We consider the 50×50 matrix having eigenvalues $\lambda_j = j$, $\lambda_{3+j} = \lambda_j + 10^{-1}$, $j = 1, 2, 3$, and the remaining eigenvalues $\lambda_j = j$, $j = 7, \ldots, 50$. The eigenvector perturbation is set to $\varepsilon = 10^{-4}$, while R_0 is taken to be a random (uniformly distributed in (0,1)) 3×3 matrix. Convergence histories are reported in the right plot of Figure 2.

Results are similar to those of the previous example, although here the more general constraint $p(\Lambda_2)R_0 = R_0p(\Lambda_3)(1-\varepsilon)$ is considered. In this example, the ill-conditioning of the eigenbasis significantly delays convergence at an early stage, as it can be deduced by the smoother convergence of the normal version of the matrix.

More examples, including the spectrum of a coefficient matrix stemming from the finite difference discretization of an elliptic partial differential operator, can be found in [24], where all results are in agreement with those above.

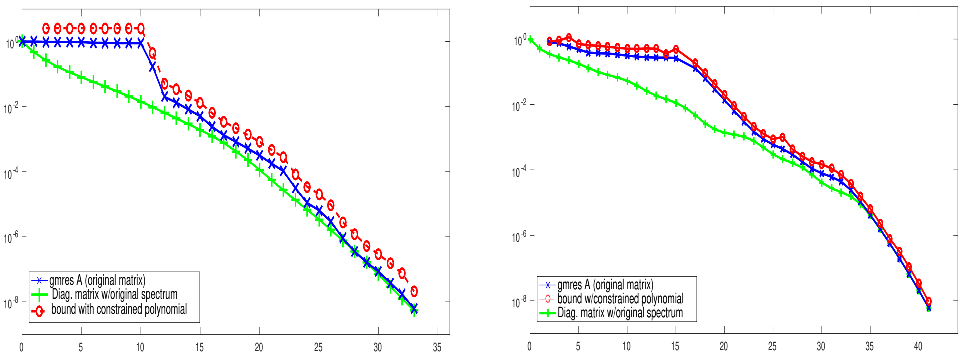

FIG. 2. GMRES *convergence history and bound from Theorem* 4.1. *Left. Example* 4.4. $R_0 = I$ *square.* $n = 50$ *complex random eigenvalues in* $(0, 10^{-2}) \times (0, 10^{-2})$*;* $\ell_3 = \ell_2 = 10$*. Right. Example* 4.5. R_0 *square with random entries,* $\ell_3 = \ell_2 = 3$*, real eigenvalues* $\lambda_j = j$*,* $j = 1, 2, 3, 7, \ldots, 50$ *and* $\lambda_{3+j} = \lambda_j + 10^{-1}$*,* $j = 1, 2, 3$.

5. The general situation. In the previous sections we assumed that most eigenvectors were orthogonal to one another. In a more generic case, many eigenvectors may be well conditioned, though not orthogonal to one other, whereas only a few of them cause the overall ill-conditioning of the eigenbasis. This occurrence can be revealed by performing a rank revealing QR factorization (RR-QR) of the eigenvector matrix. More precisely, assume that we can write the QR factors of X as

$$X = \widehat{X} R = \widehat{X} \begin{matrix} R_{11} & R_{12} & R_{13} \\ & R_{22} & R_{23} \\ & & \varepsilon R_{33} \end{matrix},$$

where $0 < \varepsilon < 1$ and $\kappa(R_{ii}) = \mathcal{O}(1)$, $i = 1, 2, 3$. To generalize the setting of the previous section, we explore how the almost linear dependence of the third block, X_3, with respect to the previous blocks, influences the overall ill-conditioning. To this end, we assume that $[X_1, X_2]$ are well conditioned, so that $\|R_{12}\| = O(1)$ or smaller. With this problem model, ill-conditioning of the basis is observed if some of the entries of $R_{i,3}$, $i = 1, 2$, are sizable, which clearly indicate a quasi-linear dependence between the last block of eigenvectors and some of the previous ones. To fix ideas, let us assume that $\|R_{23}\| \approx 1$ and $\|R_{13}\| \ll 1$, that is, linear independence between the blocks X_2 and X_3 is weak. The generalization of the argument from the previous sections suggests that the matrix blocks $R_{2,2}, R_{2,3}$, and $R_{3,3}$ have an impact on the GMRES polynomial; we next confirm this intuition. However, we will show that the ill-conditioning may also propagate to other blocks of R through inversion operations. The unitary transformation with $\widehat{X}$ allows us to detect—if present—the ill-conditioning given by part of the eigenvector basis. Following the strategy outlined in previous sections, we write that $A = X\Lambda X^{-1} = \widehat{X} R \Lambda R^{-1} \widehat{X}^H$, where

$$R^{-1} = \begin{bmatrix} R_{11}^{-1} & -R_{11}^{-1} R_{12} R_{22}^{-1} & S \\ & R_{22}^{-1} & -R_{22}^{-1} R_{23} \frac{R_{33}^{-1}}{\varepsilon} \\ & & \frac{R_{33}^{-1}}{\varepsilon} \end{bmatrix}, \quad S = -R_{11}^{-1}(R_{13} - R_{12} R_{22}^{-1} R_{23}) \frac{R_{33}^{-1}}{\varepsilon},$$

so that

$$
\begin{aligned}
p(A) &= \widehat{X}(Rp(\Lambda)R^{-1})\widehat{X}^H \\
&= \widehat{X}\begin{bmatrix} R_{11}p(\Lambda_1)R_{11}^{-1} & S_{12} & \frac{S_{13}}{\varepsilon} \\ & R_{22}p(\Lambda_2)R_{22}^{-1} & \frac{S_{23}}{\varepsilon} \\ & & R_{33}p(\Lambda_3)R_{33}^{-1} \end{bmatrix}\widehat{X}^H.
\end{aligned} \tag{5.1}
$$

Here S_{ij} are matrices depending on $R_{k\ell}$, and $p(\Lambda_k)$, $k = 1,2,3$, but not on ε. The difference from the previous section is that now ε affects not only the magnitude of the matrix polynomial block associated with the ill-conditioned portion of X, that is, the (2,3) block, but also the (1,3) block. Therefore, unless S_{13}/ε is small, further constraints are implicitly imposed on the GMRES polynomial, and convergence is likely to be delayed further.

In the following we illustrate the role of the more structured R with an example stemming from benchmark data. We consider the matrix `pores_2`, from the Matrix Market repository [19], of size $n = 1224$. The right-hand side b is the normalized vector of all ones throughout. The eigenvector matrix has condition number $\kappa(X) \approx 1.85\,10^6$. An RR-QR decomposition of the eigenvector matrix[4] shows that the last 4×4 diagonal block of the R-matrix is given by

$$
\varepsilon R_{33} = \begin{bmatrix} 3.8815e-04 & 1.9262e-18 & 2.4946e-18 & 3.6424e-05 \\ 0 & 2.1916e-04 & 1.6152e-04 & 7.8745e-17 \\ 0 & 0 & 7.4929e-06 & 1.9511e-16 \\ 0 & 0 & 0 & 2.3945e-06 \end{bmatrix}
$$

with $\varepsilon = \mathcal{O}(10^{-4})$ and $\kappa(R_{33}) \approx 1.63\,10^2$; the conditioning of $[X_1, X_2]$, that is, of the first $n-4 = 1220$ columns of X (with the ordering induced by RR-QR), is $4.6\,10^3$. If one were to consider only the last 2×2 block as εR_{33}, then $\varepsilon = \mathcal{O}(10^{-6})$ and $\kappa(R_{33}) \approx 3.13$; in this case, the conditioning of the first $n-2 = 1222$ columns of X would be $1.98\,10^4$. Therefore, the whole block X_3, that is, the last four columns of X, is responsible for the ill-conditioning of the whole basis, not just the last two columns. In the left plot of Figure 3 we report the magnitude of the diagonal elements of R, while the middle plot shows the magnitude of all elements of R that are above 10^{-2}. The right plot zooms over the last four columns of R, that is, $[R_{13}; R_{23}; \varepsilon R_{33}]$, showing that only very few selected elements are above 10^{-2}. The eigenvectors corresponding to those large row elements in $[R_{13}; R_{23}]$ are involved in the ill-conditioning of the whole basis. Figure 4 reports the matrix spectrum, with the eigenvalues corresponding to the ill-conditioned eigenvectors highlighted.

Figure 5 shows the performance of GMRES on the original matrix `pores_2` (solid line) and on a modified matrix, whose eigenvector matrix is $X = [\widehat{X}_1, \widehat{X}_2, \widetilde{X}_3]$, where $\widetilde{X}_3$ is obtained as the last block of the RR-QR decomposition after having zeroed out the elements of R_{13}, R_{23} that are below 10^{-2}. With this form, the eigenvector matrix is orthonormal except for the last four columns, so as to fit the hypotheses of the previous section. The GMRES convergence is very similar in the two cases, indicating that for this example the bound of Theorem 4.1 may apply.

Our last experiment concerns the role of the nondiagonal blocks of R: we show that if these nondiagonal blocks are sizable, the ill-conditioning of X_3 may affect the whole basis, delaying convergence. We thus applied GMRES after having modified all

[4] We use the MATLAB function `rrqrx` from the RR-QR factorization package by Ivo Houtzager; see, e.g., https://it.mathworks.com/matlabcentral/fileexchange/18591-rank-revealing-qr-factorization.

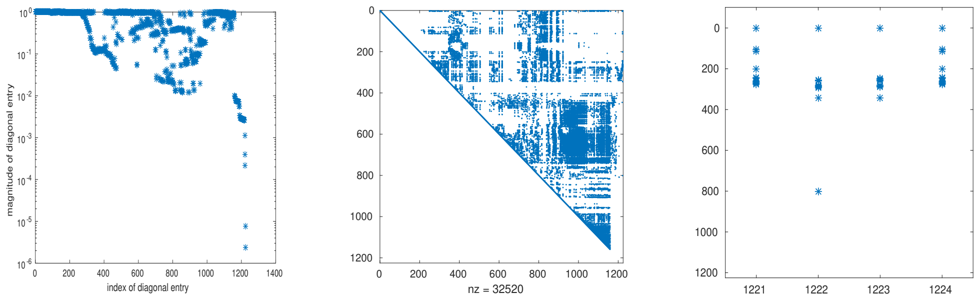

FIG. 3. *Elements of the R-matrix in the RR-QR of the* `pores_2` *eigenvector matrix. Left: diagonal elements. Middle: all elements. Right: zoom on the last four columns. (In the last two figures only the elements above* 10^{-2} *in magnitude were displayed.)*

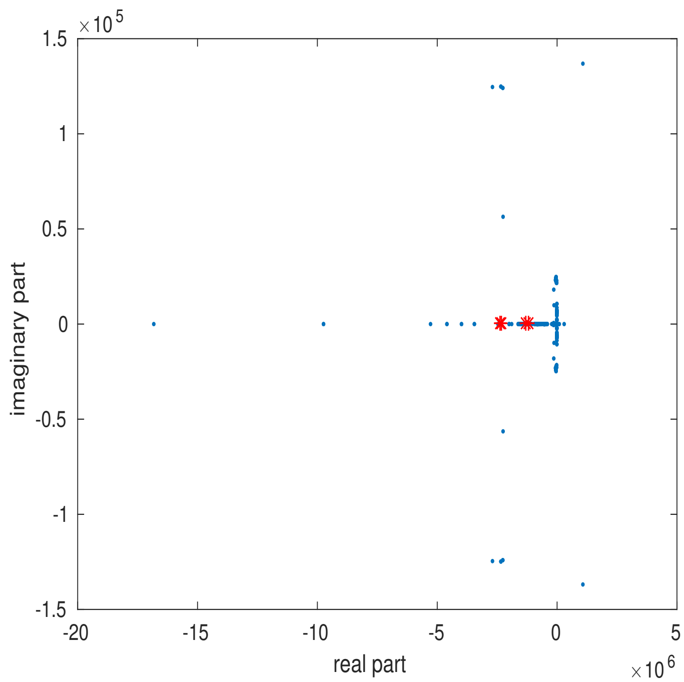

FIG. 4. *Eigenvalues of* `pores_2`*; marked "∗" are the eigenvalues corresponding to the ill-conditioned eigenvectors.*

elements in R_{13}, R_{23} to one, so that the ill-conditioning spreading effect in the matrix polynomial $p(A)$ discussed around (5.1) can be observed; note that the condition number of the whole eigenbasis did not change significantly. The worse performance with this setting is noticeable in the right plot (dashed line) of Figure 5.

6. Conclusions. We have analyzed the GMRES convergence when the eigenvectors of the coefficient matrix have a localized (block) ill-conditioning. In our analysis the GMRES residual polynomial takes care of this ill-conditioning by leveling its values among the eigenvalues of all involved eigenvectors, so as to balance the ill-conditioning. Indeed, while exploring this behavior by explicitly solving the constrained min-max problem in our numerical experiments, it often happened that `fsolve` stopped imme-

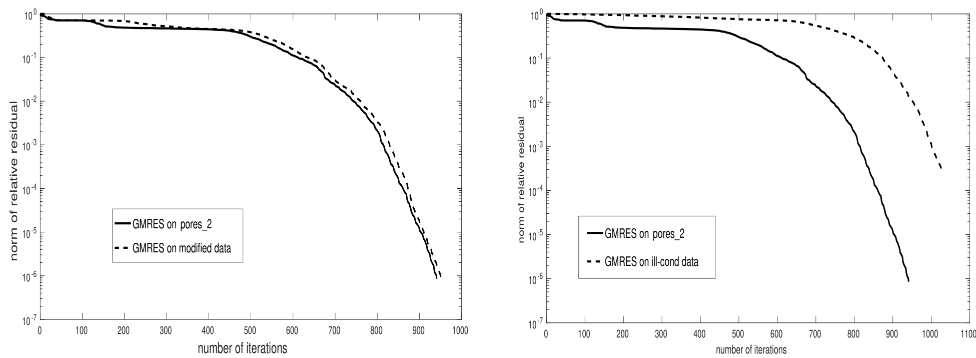

FIG. 5. GMRES *convergence history on matrix* pores_2. *Left: original matrix and modified matrix obtained by making most eigenvectors orthogonal. Right: original matrix and modified matrix obtained by spreading the ill-conditioning among all components of* $p(A)$ *(see* (5.1)*).*

diately, without doing any iteration, which means that the GMRES residual polynomial (our initial guess for the nonlinear iteration) solved the constrained minimization problem within the specified tolerances. The phenomenon supports the fact that constraints (2.7) and (4.7) not only provide a bound for the GMRES residual norms but also actually describe the GMRES residual polynomial behavior, thus providing a possible understanding of the true behavior of the GMRES polynomial. We have also experimentally shown that in the case of a more general eigenvector structure, the actual GMRES behavior may still be similar to that of localized ill-conditioning. Taken to the limit, if the whole eigenvector matrix is intrinsically ill-conditioned, our theory predicts that the GMRES polynomial should take approximately the same values throughout the spectrum, which causes a long convergence delay until this is achieved.

Appendix A. Solving the constrained minimization problem. In this appendix we discuss the numerical solution of the constrained minimization problem appearing in Theorems 2.4 and 4.1 with Remark 4.3,

$$\min_{\substack{p\in\mathbb{P}_m^* \\ p(\beta)=\frac{p(\beta)-p(\alpha)}{\varepsilon}}} \|p(\Lambda)c_0\| \qquad \text{and} \qquad \min_{\substack{p\in\mathbb{P}_m^* \\ p(\Lambda_3)=\frac{p(\Lambda_3)-p(\Lambda_2)}{\varepsilon}}} \|p(\Lambda)c_0\| . \tag{A.1}$$

We would like to stress that we do not advise actually performing these calculations during the GMRES iterations, since in our context this is only done for theoretical purposes. We use the following expression for a polynomial in $\mathbb{P}_m^*$ with known roots, $\boldsymbol{\rho} = [\rho_1, \ldots, \rho_m]^T$:

$$p(z, \boldsymbol{\rho}) = \prod_{j=1}^{m} \left(1 - \frac{z}{\rho_j}\right).$$

The GMRES residual polynomial roots, i.e., the harmonic Ritz values, have been extensively analyzed (see, e.g., [9], [22], [27, sect. 6]). If needed, these roots can be computed explicitly during the GMRES iteration by solving a generalized eigenvalue problem associated with the projection and restriction of the matrix A onto the Krylov subspace; see, e.g., [27, sect. 6]. In our experiments we used the harmonic Ritz values as an initial guess in the nonlinear iterative methods for solving the constrained problem.

We can now describe the numerical procedure for solving the constrained problem in (A.1). Identifying $\mathbb{C}$ with $\mathbb{R}^2$, we see that the function $F : \mathbb{R}^{2m} \to \mathbb{R}$ to be minimized is given by

$$F(c) := \|p(\Lambda, \boldsymbol{\rho})c_0\|^2 = \sum_{h=1}^{n} \left(\overline{p(\lambda_h, \boldsymbol{\rho}) c_0{}^{(h)}}\right) \left(p(\lambda_h, \boldsymbol{\rho}) c_0{}^{(h)}\right),$$

while the constraint function $\phi : \mathbb{R}^{2m} \to \mathbb{R}^{n_1}$, $\phi(\boldsymbol{\rho}) = (\phi_1(\boldsymbol{\rho}), \ldots, \phi_{n_1}(\boldsymbol{\rho}))^T$ has components

$$\begin{aligned}\phi_k(\boldsymbol{\rho}) :=& \left|(1-\varepsilon) p(\lambda_{n_1+k}, \boldsymbol{\rho}) - p(\lambda_k, \boldsymbol{\rho})\right|^2 \\ =& \left((1-\varepsilon)\overline{p(\lambda_{n_1+k}, \boldsymbol{\rho})} - \overline{p(\lambda_k, \boldsymbol{\rho})}\right)\left((1-\varepsilon) p(\lambda_{n_1+k}, \boldsymbol{\rho}) - p(\lambda_k, \boldsymbol{\rho})\right).\end{aligned}$$

Both F and ϕ are $\mathbb{R}$-differentiable with respect to the real and imaginary parts of the roots $\rho_j =: x_j + iy_j$, so we can address the minimization problem by making use of Lagrange multipliers, which give rise to the nonlinear system

$$\text{(A.2)} \qquad \Phi(\{x_j\}, \{y_j\}, \{\mu_k\}) = 0 \quad \Leftrightarrow \quad \begin{cases} \nabla F(\boldsymbol{\rho}) - \displaystyle\sum_{k=1}^{n_1} \mu_k \nabla \phi_k(\boldsymbol{\rho}) = 0, \\ \phi(\boldsymbol{\rho}) = 0 \end{cases}$$

with $\Phi : \mathbb{R}^{2m+n_1} \to \mathbb{R}^{2m+n_1}$ in the unknowns x_j, y_j, and μ_k for $j = 1, \ldots, m$ and $k = 1, \ldots, n_1$.

To solve $\Phi(s) = 0$ we used the MATLAB built-in function `fsolve` that implements several globally convergent Newton-like variants. The results we report in this paper were obtained through both the Trust-Region Dogleg and the Levenberg–Marquardt algorithms (depending on which behaved best in terms of convergence and stability) [21].

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