THE FIELD OF VALUES BOUNDS ON IDEAL GMRES

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Abstract. A widely known result of Elman, and its improvements due to Starke, Eiermann and Ernst, gives a bound on the worst-case GMRES residual norm using quantities related to the field of values of the given matrix and its inverse. We prove that these bounds also hold for the ideal GMRES approximation, and we derive some improvements of the bounds.

 ${\bf Key}$ words. GMRES method, convergence bounds, worst-case GMRES, ideal GMRES, field of values

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1. Introduction. Consider a linear algebraic system Ax = b with a nonsingular matrix $A \in \mathbb{F}^{n \times n}$ and a right hand side $b \in \mathbb{F}^n$, where $\mathbb{F} = \mathbb{R}$ or $\mathbb{F} = \mathbb{C}$. Given an initial approximation $x_0 \in \mathbb{F}^n$ and the initial residual $r_0 \equiv b - Ax_0$, the GMRES method of Saad and Schultz [25] iteratively constructs approximations x_k such that

$$||r_k|| = ||b - Ax_k|| = \min_{p \in \pi_k(\mathbb{F})} ||p(A)r_0||, \quad k = 1, 2, \dots,$$
(1.1)

where $||v|| \equiv \langle v, v \rangle^{1/2}$ denotes the Euclidean norm on \mathbb{F}^n , and $\pi_k(\mathbb{F})$ is the set of polynomials p of degree at most k with coefficients in \mathbb{F} , and with p(0) = 1.

The convergence analysis of GMRES has been a challenge since the introduction of the algorithm; see [19] or [18, Section 5.7] for surveys of this research area. Here we focus on GMRES convergence bounds that are independent of the initial residual, i.e., for a given A, we consider the worst-case behavior of the method. It is easy to see that for each given A, b and x_0 , the kth relative GMRES residual norm satisfies

$$\frac{\|r_k\|}{\|r_0\|} \le \max_{\substack{v \in \mathbb{F}^n \\ \|v\|=1}} \min_{p \in \pi_k(\mathbb{F})} \|p(A)v\|.$$
(1.2)

The expression on the right hand side is called the kth worst-case GMRES residual norm. For each given matrix A and iteration step k, this quantity is attainable by the relative GMRES residual norm for some initial residual r_0 . Mathematical properties of worst-case GMRES have been studied in [11]; see also [20].

Let $\mathbb{F} = \mathbb{R}$ and let $M \equiv \frac{1}{2}(A + A^T)$ be the symmetric part of A. Assuming that M is positive definite, a widely known result of Elman, stated originally for the relative residual norm of the GCR method in [9, Theorem 5.4 and 5.9], implies that

$$\max_{\substack{v \in \mathbb{R}^n \\ \|v\| = 1}} \min_{p \in \pi_k(\mathbb{R})} \|p(A)v\| \le \left(1 - \frac{\lambda_{\min}(M)^2}{\lambda_{\max}(A^T A)}\right)^{k/2};$$
(1.3)

see also the paper [8, Theorem 3.3].

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Let $\mathcal{F}(A)$ be the field of values of $A \in \mathbb{F}^{n \times n}$, and let $\nu(A)$ be the distance of $\mathcal{F}(A)$ from the origin, i.e.,

$$\mathcal{F}(A) \equiv \{ \langle Av, v \rangle : v \in \mathbb{C}^n, \|v\| = 1 \}, \quad \nu(A) \equiv \min_{z \in \mathcal{F}(A)} \|z\|.$$

Then the bound (1.3) can be written as

$$\max_{\substack{v \in \mathbb{R}^n \\ \|v\|=1}} \min_{p \in \pi_k(\mathbb{R})} \|p(A)v\| \le \left(1 - \frac{\nu(A)^2}{\|A\|^2}\right)^{k/2}.$$
(1.4)

It can be easily shown (see [3]), that the bound (1.4) holds for general nonsingular matrices $A \in \mathbb{C}^{n \times n}$, without any assumption on the Hermitian part of A.

Starke proved in [26, Section 2.2] and the subsequent paper [27, Theorem 3.2], that if $A \in \mathbb{R}^{n \times n}$ has a positive definite symmetric part M, then

$$\max_{\substack{v \in \mathbb{R}^n \\ \|v\|=1}} \min_{p \in \pi_k(\mathbb{R})} \|p(A)v\| \le \left(1 - \nu(A)\nu(A^{-1})\right)^{k/2}.$$
(1.5)

For a general nonsingular matrix we have

$$\frac{\nu(A)}{\|A\|^2} \le \min_{w \in \mathbb{C}^n \setminus \{0\}} \left| \frac{\langle Aw, w \rangle}{\langle w, w \rangle} \frac{\langle w, w \rangle}{\langle Aw, Aw \rangle} \right| = \min_{v \in \mathbb{C}^n \setminus \{0\}} \left| \frac{\langle A^{-1}v, v \rangle}{\langle v, v \rangle} \right| = \nu(A^{-1}), \quad (1.6)$$

which yields

$$1 - \nu(A)\nu(A^{-1}) \le 1 - \frac{\nu(A)^2}{\|A\|^2}.$$

Hence, as pointed out by Starke in [26, 27], the bound (1.5) improves Elman's bound (1.3). In [7, Corollary 6.2], Eiermann and Ernst proved that the bound (1.5) holds for any nonsingular matrix $A \in \mathbb{C}^{n \times n}$. In particular, no assumption on the Hermitian part of A is required. Note, however, that the bound (1.5) provides some information about the convergence of (worst-case) GMRES only when $0 \notin \mathcal{F}(A)$, or, equivalently, $0 \notin \mathcal{F}(A^{-1})$.

In many situations the convergence of GMRES and even of worst-case GMRES is superlinear, and therefore linear bounds like (1.4) and (1.5) may significantly overestimate the (worst-case) GMRES residual norms. Nevertheless, such bounds can be very useful in the practical analysis of the GMRES convergence, since they depend only on simple properties of the matrix A, which may be estimated also in complicated applications. For example, Starke used his bound in [26, 27] to analyze the dependence of the convergence of hierarchical basis and multilevel preconditioned GMRES applied to finite element discretized elliptic boundary value problems on the mesh size and the size of the skew-symmetric part of the preconditioned discretized operator. Similarly, Elman's bound was used in the analysis of the GMRES convergence for finite element discretized elliptic boundary value problems that are preconditioned with additive and multiplicative Schwarz methods [4, 5]. Many further such applications exist.

A straightforward upper bound on the *k*th worst-case GMRES residual norm is given by the *k*th *ideal GMRES approximation*, originally introduced in [14],

$$\max_{\substack{v \in \mathbb{P}^n \\ |v\|=1}} \min_{p \in \pi_k(\mathbb{F})} \|p(A)v\| \leq \min_{\substack{p \in \pi_k(\mathbb{F}) \\ \|v\|=1}} \max_{\substack{v \in \mathbb{P}^n \\ \|v\|=1}} \|p(A)v\| = \min_{\substack{p \in \pi_k(\mathbb{F}) \\ \text{ideal GMRES}}} \|p(A)\|.$$
(1.7)

As shown by examples in [10, 29] and more recently in [11], there exist matrices A and iteration steps k for which the inequality in (1.7) can be strict. The example in [29] even shows that the ratio of worst-case and ideal GMRES can be arbitrarily small. A survey of the mathematical relations between the two approximation problems in (1.7) is given in the introductory sections of [28].

The main goal in this paper is to show that the right hand side of the bound (1.5) also represents an upper bound on the ideal GMRES approximation for general (nonsingular) complex matrices. This has been stated without proof already in our paper [19, p. 168] and later in the book [18, Section 5.7.3]. In light of the practical relevance of Elman's and Starke's bounds, and of the fact that the inequality in (1.7) can be strict, we believe that providing a complete proof is important. This proof and a further discussion of the bounds are given in Section 2. In Section 3 we derive some improvements of the considered bounds.

Throughout the rest of this paper we will consider the general setting with $\mathbb{F} = \mathbb{C}$.

2. Proof of the ideal GMRES bound. Consider a nonsingular matrix $A \in \mathbb{C}^{n \times n}$, a unit norm vector $v \in \mathbb{C}^n$, and the minimization problem

$$\min_{\alpha \in \mathbb{C}} \|v - \alpha A v\|^2.$$

It is easy to show that the minimum is attained for

$$\alpha_* \equiv \frac{\langle v, Av \rangle}{\langle Av, Av \rangle}$$

and that

$$\|v - \alpha_* Av\|^2 = 1 - \frac{\langle Av, v \rangle}{\langle v, v \rangle} \frac{\langle v, Av \rangle}{\langle Av, Av \rangle}.$$
(2.1)

Another result we will use below is that ideal and worst-case GMRES for any matrix $A \in \mathbb{C}^{n \times n}$ are equal in the iteration step k = 1, i.e.,

$$\min_{\alpha \in \mathbb{C}} \max_{\substack{v \in \mathbb{C}^n \\ \|v\|=1}} \|v - \alpha Av\| = \max_{\substack{v \in \mathbb{C}^n \\ \|v\|=1}} \min_{\alpha \in \mathbb{C}} \|v - \alpha Av\|;$$
(2.2)

see [17, Theorem 1] and [13, Theorem 2.5]. This equality has also been shown in the context of bounded linear operators on a Hilbert space; see [1] or [15, Section 3.2] and the references given there.

After these preparations we can now state and prove our main result.

THEOREM 2.1. If $A \in \mathbb{C}^{n \times n}$ is nonsingular, then for all $k \geq 1$ we have

$$\min_{p \in \pi_k(\mathbb{C})} \|p(A)\| \le \left(1 - \nu(A)\nu(A^{-1})\right)^{k/2}.$$
(2.3)

Moreover, if $M = \frac{1}{2}(A + A^H)$ is positive definite, then

$$\min_{p \in \pi_k(\mathbb{C})} \|p(A)\| \le \left(1 - \frac{\lambda_{\min}(M)^2}{\lambda_{\max}(A^H A)}\right)^{k/2}.$$
(2.4)

Proof. The ideal GMRES approximation satisfies

$$\min_{p \in \pi_k(\mathbb{C})} \|p(A)\| \le \min_{\alpha \in \mathbb{C}} \|(I - \alpha A)^k\| \le \min_{\alpha \in \mathbb{C}} \|I - \alpha A\|^k.$$
(2.5)

Using (2.2) and (2.1) we then get

$$\begin{split} \min_{\alpha \in \mathbb{C}} \|I - \alpha A\|^{k} &= \min_{\substack{v \in \mathbb{C}^{n} \\ \|v\|=1}} \max_{v \in \mathbb{C}^{n}} \|v - \alpha Av\|^{k} = \max_{\substack{v \in \mathbb{C}^{n} \\ \|v\|=1}} \min_{\alpha \in \mathbb{C}} \|v - \alpha Av\|^{2} \\ &= \max_{\substack{v \in \mathbb{C}^{n} \\ \|v\|=1}} \left(\min_{\alpha \in \mathbb{C}} \|v - \alpha Av\|^{2} \right)^{k/2} \\ &= \max_{\substack{v \in \mathbb{C}^{n} \\ \|v\|=1}} \left(1 - \frac{\langle Av, v \rangle}{\langle v, v \rangle} \frac{\langle v, Av \rangle}{\langle Av, Av \rangle} \right)^{k/2} \\ &= \left(1 - \min_{\substack{v \in \mathbb{C}^{n} \\ \|v\|=1}} \frac{\langle Av, v \rangle}{\langle v, v \rangle} \frac{\langle v, Av \rangle}{\langle Av, Av \rangle} \right)^{k/2} \\ &\leq \left(1 - \min_{\substack{v \in \mathbb{C}^{n} \\ \|v\|=1}} \left| \frac{\langle Av, v \rangle}{\langle v, v \rangle} \right| \min_{w \in \mathbb{C}^{n} \setminus \{0\}} \left| \frac{\langle A^{-1}w, w \rangle}{\langle w, w \rangle} \right| \right)^{k/2} \\ &= \left(1 - \nu(A)\nu(A^{-1}) \right)^{k/2}, \end{split}$$
(2.6)

which proves (2.3). If $M = \frac{1}{2}(A + A^H)$ is positive definite, then $\lambda_{\min}(M) \leq \nu(A)$ and

$$\frac{\lambda_{\min}(M)}{\lambda_{\max}(A^H A)} \le \nu(A^{-1})$$

(see (1.6)), and then (2.3) implies (2.4).

The derivation of the bound (2.3) involves several inequalities, which are usually not tight; see (2.5) and (2.6). We therefore can expect that the right hand side of (2.3) is in most cases much larger than the left hand side.

Since $0 \leq \nu(A)\nu(A^{-1}) \leq 1$ holds for every matrix $A \in \mathbb{C}^{n \times n}$, equality holds in (2.3) when the ideal GMRES approximation stagnates until the iteration step k, i.e., when

$$\min_{p \in \pi_k(\mathbb{C})} \|p(A)\| = 1.$$
(2.7)

For this to happen it is necessary that $0 \in \mathcal{F}(A) \Leftrightarrow 0 \in \mathcal{F}(A^{-1})$, and it is necessary and sufficient that

 $0 \in \{z \in \mathbb{C} : ||p(A)|| \ge |p(z)| \text{ for all complex polynomials } p \text{ of degree } \le k\}.$

More information about the relation between the *polynomial numerical hull* (i.e. the set stated above) and the stagnation of ideal GMRES can be found in [10, 12]. The (complete) stagnation of GMRES, which implies the stagnation of worst-case and ideal GMRES has been analyzed, for example, in [20, 22, 30].

We can also identify some cases when one of the inequalities in (2.5) is an equality. First note that if the left hand side of (2.5) is larger than zero, then the polynomial solving this minimization problem, i.e., the *k*th ideal GMRES polynomial, is unique; see [14, 21]. Hence, in this case the first inequality in (2.5) is an equality if and only if the *k*th ideal GMRES polynomial is of the form $(1 - \alpha z)^k$. One of the very rare cases where this happens without stagnation is when $A = J_\lambda$ is an $n \times n$ Jordan block with a sufficiently large eigenvalue $\lambda > 0$ and $1 \le k < n/2$; see [28, Theorem 3.2] for details. The *k*th ideal GMRES polynomial then is $(1 - \lambda^{-1}z)^k$, and we obtain

$$\min_{p \in \pi_k(\mathbb{C})} \| p(J_{\lambda}) \| = \| (I - \lambda^{-1} J_{\lambda})^k \| = \lambda^{-k} = \| I - \lambda^{-1} J_{\lambda} \|^k.$$

In this special case also the second inequality in (2.5) is an equality. For a more general (sufficient) criterion for equality, recall that a matrix $X \in \mathbb{C}^{n \times n}$ is called *radial* when its *numerical radius* is equal to its 2-norm, i.e.,

$$r(X) \equiv \max_{z \in \mathcal{F}(X)} |z| = ||X||.$$
(2.8)

This holds if and only if $||X^k|| = ||X||^k$ for all $k \ge 1$. Several other equivalent characterizations of this property are given in [16, Problem 27, p. 45]; see also [24]. Suppose that the matrix $I - \tilde{\alpha}A$ is radial for some $\tilde{\alpha} \in \mathbb{C}$ that solves the minimization problem $\min_{\alpha \in \mathbb{C}} ||(I - \alpha A)^k||$. Then

$$\min_{\alpha \in \mathbb{C}} \|I - \alpha A\|^k \ge \min_{\alpha \in \mathbb{C}} \|(I - \alpha A)^k\| = \|(I - \widetilde{\alpha} A)^k\| = \|I - \widetilde{\alpha} A\|^k \ge \min_{\alpha \in \mathbb{C}} \|I - \alpha A\|^k,$$

which shows that equality holds throughout and hence also in the second inequality in (2.5).

Finally, it is clear that in most cases the inequality (2.6) will be strict: When solving

$$\min_{\substack{v \in \mathbb{C}^n \\ \|v\| = 1}} \frac{\langle Av, v \rangle}{\langle v, v \rangle} \frac{\langle v, Av \rangle}{\langle Av, Av \rangle} = \min_{\substack{v \in \mathbb{C}^n \\ \|v\| = 1}} \left(\frac{|\langle Av, v \rangle|}{\|v\| \|Av\|} \right)^2 = \min_{v \in \mathbb{C}^n} \cos^2 \angle (v, Av)$$

we try to make the vectors v and Av as close as possible to orthogonal, and hence only the angle between the vectors plays a role. On the other hand, solutions of

$$\min_{v \in \mathbb{C}^n \atop \|v\| = 1} \left| \frac{\langle Av, v \rangle}{\langle v, v \rangle} \right| \quad \text{and} \quad \min_{w \in \mathbb{C}^n \setminus \{0\}} \left| \frac{\langle A^{-1}w, w \rangle}{\langle w, w \rangle} \right|$$

depend on the cosine of the angle as well as on the length of the vectors.

3. An improvement of Theorem 2.1. Using the numerical radius defined in (2.8), we can write

$$\nu(A^{-1})r(A) = \min_{v \in \mathbb{C}^n \setminus \{0\}} \left| \frac{\langle v, Av \rangle}{\langle Av, Av \rangle} \right| \max_{v \in \mathbb{C}^n \atop \|v\| = 1} |\langle Av, v \rangle|.$$

If $w \in \mathbb{C}^n$ is a unit norm vector that maximizes $|\langle Av, v \rangle|$, then

$$\min_{v \in \mathbb{C}^n \setminus \{0\}} \left| \frac{\langle v, Av \rangle}{\langle Av, Av \rangle} \right| \max_{\substack{v \in \mathbb{C}^n \\ \|v\| = 1}} |\langle Av, v \rangle| \le \left| \frac{\langle w, Aw \rangle}{\|Aw\|} \right| \left| \frac{\langle Aw, w \rangle}{\|Aw\|} \right| \le 1,$$

so that $\nu(A^{-1}) \leq 1/r(A)$. If we define $\beta \in (0, \frac{\pi}{2})$ by

$$\cos\beta = \frac{\nu(A)}{r(A)},\tag{3.1}$$

we obtain

$$1 - \cos\beta \le 1 - \nu(A)\nu(A^{-1}). \tag{3.2}$$

It is tempting to think that the quantity $1 - \cos \beta$ yields an improvement of the bound (2.3). As shown in the following example, however, this is not the case.

EXAMPLE. Consider the matrix

$$A = \begin{bmatrix} \lambda & 1\\ 0 & \lambda \end{bmatrix} \in \mathbb{R}^{2 \times 2} \quad \text{with} \quad \lambda > \frac{1}{2}.$$

We have n = 2 and we are interested in the iteration step k = 1. The set $\mathcal{F}(A)$ is a disk with center at λ and radius $\frac{1}{2}$ (independent of λ), so that

$$\nu(A) = \lambda - \frac{1}{2}, \quad r(A) = \lambda + \frac{1}{2}, \quad (1 - \cos \beta)^{1/2} = \frac{1}{\sqrt{\lambda + \frac{1}{2}}}$$

Using [28, Example 2] for n = 2 and k = 1,

$$\min_{\alpha \in \mathbb{R}} \|I - \alpha A\| = \frac{1}{\lambda + \frac{1}{4\lambda}}.$$

For the particular value $\lambda = \frac{2}{3}$ we get

$$(1 - \cos\beta)^{1/2} = \left(\frac{6}{7}\right)^{1/2} \approx 0.9258 < 0.96 = \min_{\alpha \in \mathbb{R}} \|I - \alpha A\|.$$

The bound (2.3) on the other hand holds with $(1 - \nu(A^{-1})\nu(A))^{1/2} = (15/16)^{1/2} \approx 0.9682.$

Next note that for any matrix $A \in \mathbb{C}^{n \times n}$ with $0 \notin \mathcal{F}(A)$ we have, possibly after a suitable rotation that can be done without loss of generality, the inclusion

$$\mathcal{F}(A) \subseteq \{ z : \operatorname{Re}(z) \ge r(A) \cos \beta \} \cap \{ |z| \le r(A) \}.$$

This inclusion is potentially tighter than the one used by Beckermann, Goreinov and Tyrtyshnikov in [3], which is based on ||A|| instead of r(A). (Recall that $r(A) \leq ||A|| \leq 2r(A)$ holds for any matrix $A \in \mathbb{C}^{n \times n}$.) Using the same techniques as in [3], and exploiting also that

$$||p(A)|| \le (1 + \sqrt{2}) ||p||_{\mathcal{F}(A)}$$

holds for any complex polynomial p (see [6]), we therefore obtain the following improved version of [3, Theorem 2.1].

THEOREM 3.1. If $A \in \mathbb{C}^{n \times n}$ is such that $0 \notin \mathcal{F}(A)$, and $\beta \in (0, \frac{\pi}{2})$ is given as in (3.1), then for all $k \geq 1$ we have

$$\min_{p \in \pi_k(\mathbb{C})} \|p(A)\| \le (1 + \sqrt{2})(2 + \rho_\beta)\rho_\beta^k < 8\rho_\beta^k,$$
(3.3)

where $\rho_{\beta} \equiv 2 \sin\left(\frac{\beta}{4-2\beta/\pi}\right) < \sin\beta$.

Now suppose that $A \in \mathbb{C}^{n \times n}$ is such that $0 \notin \mathcal{F}(A)$ and that, possibly after a suitable rotation, the set $\mathcal{F}(A)$ is contained in a disk D with center c and radius δ given by

$$c = \frac{\nu(A) + r(A)}{2}$$
, and $\delta = \frac{r(A) - \nu(A)}{2}$. (3.4)

It has been shown in [2], based on results [23], that if $\mathcal{F}(A) \subseteq D$, then

$$||p(A)|| \le 2 \max_{z \in D} |p(z)|$$

holds for any polynomial p. Moreover, it is well known that the problem

$$\min_{p \in \pi_k(\mathbb{C})} \max_{z \in D} |p(z)|$$

is solved by the polynomial $(1 - \frac{1}{c}z)^k$. This yields the following improvement of Theorem 2.1.

LEMMA 3.2. If $A \in \mathbb{C}^{n \times n}$ is such that $0 \notin \mathcal{F}(A) \subseteq D$ as stated above, and $\beta \in (0, \frac{\pi}{2})$ is given as in (3.1), then for all $k \geq 1$ we have

$$\min_{p \in \pi_k(\mathbb{C})} \|p(A)\| \le 2 \left(\frac{1 - \cos\beta}{1 + \cos\beta}\right)^k < 2(1 - \nu(A)\nu(A^{-1}))^k.$$
(3.5)

Proof. We have

$$\begin{split} \min_{p \in \pi_k(\mathbb{C})} \|p(A)\| &\leq 2 \min_{p \in \pi_k(\mathbb{C})} \max_{z \in D} |p(z)| = 2 \max_{z \in D} \left| 1 - \frac{1}{c} z \right|^k = 2 \left(\frac{\delta}{c} \right)^k \\ &= 2 \left(\frac{r(A) - \nu(A)}{r(A) + \nu(A)} \right)^k \\ &= 2 \left(\frac{1 - \cos \beta}{1 + \cos \beta} \right)^k \\ &\leq 2(1 - \cos \beta))^k \\ &\leq 2(1 - \nu(A)\nu(A^{-1}))^k, \end{split}$$

where in the last inequality we have used (3.2).

The bound in Lemma 3.2 with the convergence factor

$$\frac{1 - \cos\beta}{1 + \cos\beta}$$

reminds of the error bound for the classical Richardson iteration or the steepest descent method; see, e.g., [18, Section 5.5.2]. In particular, if A is Hermitian positive definite, then $\cos \beta = \lambda_{\min}(A)/\lambda_{\max}(A) = 1/\kappa(A)$.

Also note that for any $\beta \in (0, \frac{\pi}{2})$ we have

$$\frac{1-\cos(\beta)}{1+\cos(\beta)} < 2\sin\left(\frac{\beta}{4-\frac{2}{\pi}\beta}\right),$$

which can be verified using a mathematical software, or by a more detailed analysis. Consequently, the convergence factor in Lemma 3.2 is smaller than the convergence factor in Theorem 3.1, which however is valid whenever $0 \notin \mathcal{F}(A)$.

For a numerical illustration of the bounds considered in this paper we use a single Jordan block J_{λ} of the size n = 100 and with the eigenvalue $\lambda = 3$. In Figure 3.1 we plot for the first 49 iterations the value of the ideal GMRES approximation (known to be λ^{-k} in this case), Elman's bound (1.3), Starke's bound (1.5), the improved



FIG. 3.1. Ideal GMRES and the bounds considered in this paper for a 100×100 Jordan block with the eigenvalue 3.

Beckermann-Goreinov-Tyrtyshnikov bound (3.3), and the disk bound, i.e., the first expression in (3.5). We observe that the convergence factors which determine the bounds can be quite different from each other, even in this simple case. The disk bound is by far the best, which is due to the fact that $\mathcal{F}(J_{\lambda})$ actually is a disk centered at λ .

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