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ADAPTIVE K-STEP ITERATIVE METHODS FOR NONSYMMETRIC SYSTEMS OF LINEAR EQUATIONS *

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Dedicated to Professor W. Niethammer on the occasion of his 60th birthday.

Abstract. This study is concerned with k-step methods for the iterative solution of nonsymmetric systems of real linear equations. These are generalizations of the Chebyshev (2-step) iteration, with the potential for faster convergence in cases where the spectrum of the underlying coefficient matrix is not approximated well by an ellipse. We investigate the problem of optimizing the associated (asymptotic) convergence factor with respect to a finite number of points (e.g., eigenvalue estimates obtained from using the Arnoldi process). We formulate this minimization problem as an optimization problem with constraints and propose an algorithm to compute near-best k-step parameters. The computational advantages of the Chebyshev method, such as avoidance of inner products, the implementation as an adaptive method, and the simplicity of the overall scheme, carry over to the case $k > 2$.

Key words. k-step method, Chebyshev method, adaptive implementation, polynomial iteration.

AMS subject classification. 65F10.

1. Introduction. Many problems in scientific computing frequently lead to large nonsymmetric systems of real linear equations

$$Ax = \mathbf{b}\,, \tag{1.1}$$

where it is desirable, in the numerical solution of this equation, that A, a nonsingular matrix in $\mathbf{R}^{N\times N}$, enters the computation only in the form of matrix-vector-multiplications. The usual reason for this is that A is sparse, structured, or has some other special form that can be exploited when multiplying A with a vector. This leads to the class of polynomial iterative methods, i.e., starting from an initial vector guess $\mathbf{x}_0$, the vector iterates can be expressed as

$$\mathbf{x}_n := \mathbf{x}_0 + \varphi_{n-1}(A)\mathbf{r}_0, \tag{1.2}$$

where φ_{n-1} is a polynomial of degree $n-1$ (written $\varphi_{n-1} \in \Pi_{n-1}$), and where $\mathbf{r}_0 := \mathbf{b} - A\mathbf{x}_0$ denotes the initial residual vector. From (1.2), the corresponding relation for the residual vectors,

$$\mathbf{r}_n := \mathbf{b} - A\mathbf{x}_n = (I - A\varphi_{n-1}(A))\mathbf{r}_0 = \psi_n(A)\mathbf{r}_0, \tag{1.3}$$

is obtained, and ψ_n, in Π_n with $\psi_n(0) = 1$, is called the residual polynomial associated with the iterative method.

Besides the large class of algorithms that construct appropriate residual polynomials in the course of the iteration based on certain orthogonality relations, there are the so-called Chebyshev-like methods. Since inner products constitute a bottleneck on vector and parallel computers, and since one either has to deal with recurrences that become longer during the iteration (such as in the GMRES method of Saad and Schultz [19]) or lose optimality, the development of so-called hybrid algorithms has become of interest in recent years. These hybrid algorithms perform a number of steps of some inner-product-based iteration, and then repeatedly apply a residual polynomial ψ_n,

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constructed from the information collected during this first phase. That is, once an appropriate residual polynomial ψ_n is found, the iteration proceeds as

$$\mathbf{r}_{nl} = (\psi_n(A))^{l-1}\mathbf{r}_n \quad (l = 1, 2, \ldots). \tag{1.4}$$

A popular example of this is the hybrid GMRES algorithm by Nachtigal, Reichel and Trefethen [15]. For a survey of the recent development on hybrid iterative methods, see also [14].

In contrast to this, for k a positive integer, the iterates of a k-step method are computed by a relation of the form

$$\mathbf{x}_j = \mu_0^{(j)}\mathbf{r}_{j-1} + \mu_1^{(j)}\mathbf{x}_{j-1} + \cdots + \mu_k^{(j)}\mathbf{x}_{j-k}\,. \tag{1.5}$$

A well-known example of a 2-step method is the Chebyshev iteration of Golub and Varga [7], and its extension to nonsymmetric matrices [11]. The iteration parameters $\mu_0^{(j)}, \mu_1^{(j)}, \ldots, \mu_k^{(j)}$ in (1.5) are to be determined from information obtained during the inner-product-based starting phase of the method. Our main purpose in this paper is to develop a practical algorithm which simultaneously determines a near-best value of the parameter k in the k-step method of (1.5), along with its associated parameters $\{\mu_i^{(j)}\}_{i=0}^k$ of (1.5). (The near-best determination of the parameter k will be based on certain "cost factors", associated with the iteration of (1.5), and will be discussed in Section 5.)

An important advantage of k-step methods over hybrid polynomial methods is that the corresponding residual polynomials are not restricted to products of polynomials of a *given* degree. To give an idea of the effect this subtle difference can have on the convergence factor of the associated iterative methods, consider for the moment the well-studied classical case of Chebyshev polynomials on a real interval $[\alpha, \beta]$ with $0 < \alpha < \beta$ (cf. [23, Section 5.1]). If we apply the (properly scaled and shifted) Chebyshev polynomial

$$\psi_m(x) := \frac{T_m(\frac{\beta+\alpha-2x}{\beta-\alpha})}{T_m(\frac{\beta+\alpha}{\beta-\alpha})}$$

of degree m in a cyclic fashion, then, after s such cycles, one gets an error reduction of

$$\max_{x\in[\alpha,\beta]} |\psi_m(x)|^s = \frac{2^s}{\left[\left(\frac{\sqrt{\beta}-\sqrt{\alpha}}{\sqrt{\beta}+\sqrt{\alpha}}\right)^m + \left(\frac{\sqrt{\beta}+\sqrt{\alpha}}{\sqrt{\beta}-\sqrt{\alpha}}\right)^m\right]^s}\,.$$

In contrast, on using the familiar 3-term recurrence relations for the Chebyshev polynomials, and on implementing it as a 2-step method ([23, p. 138]), we obtain the Chebyshev polynomial of degree ms, whose associated error reduction is given by

$$\max_{x\in[\alpha,\beta]} |\psi_{ms}(x)| = \frac{2}{\left(\frac{\sqrt{\beta}-\sqrt{\alpha}}{\sqrt{\beta}+\sqrt{\alpha}}\right)^{ms} + \left(\frac{\sqrt{\beta}+\sqrt{\alpha}}{\sqrt{\beta}-\sqrt{\alpha}}\right)^{ms}}\,.$$

The last error bound is *always* better (from the min-max nature of best approximation), for any $s > 1$, than that of the previous error bound, and is clearly much smaller for large values of s.

Another point that led us to this study of k-step methods is the fact, from (1.5), that we only have to treat $k+1$ parameters throughout the iterative process that implicitly constructs residual polynomials of *arbitrarily* high degree. We present here an approach for constructing such inner-product-free iterative methods.

In Section 2, we will review the theory of (non-stationary) k-step methods which was developed by Niethammer and Varga [16], Eiermann, Niethammer and Varga [4] and Eiermann [3]. The generalization to (k, l)-step methods, where not only the recent k iterates but also $l+1$ residuals are used to define the new iterate, was introduced by Parsons [17]. A detailed analysis of these methods was given by Gutknecht in [8], and a (k, l)-step adaptive algorithm, based on SCPACK [22], was proposed and tested by Li [10]. We will restrict ourselves here to k-step methods, i.e., to $l = 0$, and we note that the extension of our results and algorithms to the case $l > 0$ is mostly straightforward.

Section 3 presents an algorithm for the computation of nearly optimal k-step parameters associated with a given finite set of points, these points being presumably eigenvalue estimates obtained from Arnoldi's method. We will discuss in Section 4 the issue of implementing the iteration as an adaptive scheme. This means that, from time to time, it may be necessary to change the parameters, according to newly obtained information during the iteration process. Section 5 contains our computational experiments and, finally, in Section 6 we draw some conclusions from our experience with k-step methods.

2. Theory of k-step Methods. We start this section with a review of the theory for (non-stationary) k-step methods developed in Niethammer and Varga [16], Eiermann, Niethammer and Varga [4] and Eiermann [3]. Our k-step methods will be based on the recurrence relations for Faber polynomials associated with the function

$$\Psi_k(w) = cw + c_0 + \frac{c_1}{w} + \cdots + \frac{c_{k-1}}{w^{k-1}}. \tag{2.1}$$

Here, we assume that $c, c_0, \cdots c_{k-1}$ are given real parameters, and to avoid degeneracies here, we further assume that

$$c \neq 0 \text{ and } c_{k-1} \neq 0.$$

For $k \geq 2$, set $\rho_0 := \max\{|w| : \Psi_k'(w) = 0\}$, so that $0 < \rho_0 < \infty$, and set $\partial\Omega_k(\rho_0) := \{z = \Psi_k(w) : |w| = \rho_0\}$. If $\Omega_k(\rho_0)$ denotes the compact set in the z-plane, consisting of the union of $\partial\Omega_k(\rho_0)$ and its interior, then $\Omega_k(\rho_0)$ consists of more than one point and possesses a simply connected complement. It follows that Ψ_k maps $\{w \in \mathbb{C} : |w| > \rho_0\}$ conformally onto the exterior of $\Omega_k(\rho_0)$, with $\Psi_k(\infty) = \infty$ and $\Psi_k'(\infty) = c \neq 0$. (For $k = 1$ where $\rho_0 := 0$, similar remarks can be made.) For any $\rho > \rho_0$ the image of the circle $\{w \in \mathbb{C} : |w| = \rho\}$ will be a Jordan curve, which we denote by $\partial\Omega_k(\rho)$. We will denote $\partial\Omega_k(\rho)$ together with its interior by $\Omega_k(\rho)$. The curves $\partial\Omega_k(\rho)$ for $\rho > \rho_0$ cover the exterior of $\Omega_k(\rho_0)$, and if $\rho_1 \neq \rho_2$ where $\rho_1 > \rho_0$ and $\rho_2 > \rho_0$, then $\partial\Omega_k(\rho_1)$ and $\partial\Omega_k(\rho_2)$ are nonintersecting.

The conformal mapping $\Psi_k(w)$ generates a corresponding sequence of Faber polynomials, $\{F_m(z)\}_{m\geq 0}$ with $F_m(z) \in \Pi_m$ for each $m \geq 0$, from the generating formula (cf. Smirnov and Lebedev [20, p. 130])

$$\frac{\Psi_k'(w)}{\Psi_k(w) - z} = \sum_{m=0}^{\infty} F_m(z) w^{-m-1} \ (|w| > \rho_0, z \in \mathbb{C}),$$

which in turn, because of the special form of $\Psi_k(w)$ in (2.1), gives the following $(k+1)$-*term recurrence relation* for these Faber polynomials:

$$\begin{aligned} &F_0(z) = 1, \ F_1(z) = (z - c_0)/c, \\ &F_m(z) = [(z - c_0)F_{m-1}(z) - (c_1 F_{m-2}(z) + \ldots + c_{m-1}F_0(z)) - (m-1)c_{m-1}]/c, \\ &\quad m = 2, \ldots, k, \\ &F_m(z) = [(z - c_0)F_{m-1}(z) - (c_1 F_{m-2}(z) + \ldots + c_{k-1}F_{m-k}(z))]/c; \\ &\quad m = k+1, \ldots \end{aligned} \tag{2.2}$$

(see Henrici [9, p. 512]).

It is known (cf. Curtiss [2, p. 584]) that

$$\lim_{m\to\infty} |F_m(\Psi_k(w))|^{1/m} = |w| \tag{2.3}$$

holds uniformly on every compact subset of $\{w \in \mathbb{C} : |w| > \rho_0\}$. If we assume, in addition, that

$$0 \notin \Omega_k(\rho_0),$$

the conformal map Ψ_k, of $\{w \in \mathbb{C} : |w| > \rho_0\}$ onto the exterior of $\Omega_k(\rho_0)$, determines a unique point ω_0, satisfying $|\omega_0| > \rho_0$, for which $\Psi_k(\omega_0) = 0$, and from (2.3), it is evident that $F_m(0) \neq 0$ for all sufficiently large m. Thus, the *normalized* Faber polynomials, defined by

$$\tilde{F}_m(z) := \frac{F_m(z)}{F_m(0)} \quad \text{so that } \tilde{F}_m(0) = 1, \tag{2.4}$$

are well defined for all m sufficiently large. It turns out that these normalized Faber polynomials play a special role in applications because

$$\max_{z\in\Omega_k(\rho)} |\tilde{F}_m(z)| \leq C \min_{\psi_m\in\Pi_m, \psi_m(0)=1} \left\{ \max_{z\in\Omega_k(\rho)} |\psi_m(z)| \right\}, \tag{2.5}$$

for every $\rho \geq \rho_0$, where the constant C above depends on $\partial\Omega_k(\rho_0)$ but is independent of ρ and m (see Eiermann [3, Theorem 2], and [21, Theorems 3.1 and 3.4] for proofs of this inequality under different assumptions on $\partial\Omega_k(\rho_0)$, such as $\Omega_k(\rho_0)$ being convex or $\partial\Omega_k(\rho_0)$ being of bounded rotation). The $(k+1)$-term recurrence relation of (2.2) carries over to the vector iterates, associated with normalized Faber polynomials, as residual polynomials (cf. Eiermann [3, Lemma 1] and [21, Sect. 5]):

$$\begin{aligned} &\mathbf{x}_1 = \mu_0^{(1)}\mathbf{r}_0 + \mathbf{x}_0, \\ &\mathbf{x}_j = \mu_0^{(j)}\mathbf{r}_{j-1} + \mu_1^{(j)}\mathbf{x}_{j-1} + \cdots + \mu_j^{(j)}\mathbf{x}_0 \quad (j = 2, \ldots, k-1), \\ &\mathbf{x}_j = \mu_0^{(j)}\mathbf{r}_{j-1} + \mu_1^{(j)}\mathbf{x}_{j-1} + \cdots + \mu_k^{(j)}\mathbf{x}_{j-k} \quad (j = k, k+1, \ldots), \end{aligned} \tag{2.6}$$

where

$$\mu_0^{(1)} = \frac{1}{c_0}\,,$$

$$\mu_0^{(j)} = -\frac{1}{c}\frac{F_{j-1}(0)}{F_j(0)}\,, \mu_i^{(j)} = -\frac{c_{i-1}}{c}\frac{F_{j-i}(0)}{F_j(0)}\,,\ i = 1, \ldots, j-1\,,\ \mu_j^{(j)} = -j\frac{c_{j-1}}{c}\frac{1}{F_j(0)}$$

for $j = 2, \ldots, k$, and

$$\mu_0^{(j)} = -\frac{1}{c}\frac{F_{j-1}(0)}{F_j(0)}\,, \mu_i^{(j)} = -\frac{c_{i-1}}{c}\frac{F_{j-i}(0)}{F_j(0)} \quad (i = 1, \ldots, k), \tag{2.7}$$

for $j = k+1, \ldots$. Note that the parameters $\mu_i^{(j+1)}$ can easily be computed from the $\mu_i^{(j)}$'s, using the recurrence relation (2.2) for the $F_j(0)$'s.

The iteration (2.6) can also be written in correction-step form. First, notice that the recursion relation (2.2) yields with (2.7) that

$$\begin{aligned} &\mu_1^{(j)} + \mu_2^{(j)} + \cdots + \mu_j^{(j)} = 1 \qquad (j = 2, \ldots, k-1), \\ &\mu_1^{(j)} + \mu_2^{(j)} + \cdots + \mu_k^{(j)} = 1 \qquad (j = k, k+1, \ldots). \end{aligned} \tag{2.8}$$

Thus, we may write

$$\begin{aligned} \mathbf{x}_1 \quad &= \mathbf{x}_0 + \boldsymbol{\delta}_0\,, \\ &\boldsymbol{\delta}_0 := \mu_0^{(1)}\mathbf{r}_0\,, \\ \mathbf{x}_j \quad &= \mathbf{x}_{j-1} + \boldsymbol{\delta}_{j-1}\,, \\ &\boldsymbol{\delta}_{j-1} := \mu_0^{(j)}\mathbf{r}_{j-1} + \beta_1^{(j)}\boldsymbol{\delta}_{j-2} + \cdots + \beta_{j-1}^{(j)}\boldsymbol{\delta}_0 \qquad (j = 2, \ldots, k-1), \\ \mathbf{x}_j \quad &= \mathbf{x}_{j-1} + \boldsymbol{\delta}_{j-1}\,, \\ &\boldsymbol{\delta}_{j-1} := \mu_0^{(j)}\mathbf{r}_{j-1} + \beta_1^{(j)}\boldsymbol{\delta}_{j-2} + \cdots + \beta_{k-1}^{(j)}\boldsymbol{\delta}_{j-k} \quad (j = k, k+1, \ldots), \end{aligned} \tag{2.9}$$

where

$$\begin{aligned} &\beta_i^{(j)} := \textstyle\sum_{l=1}^{i}\mu_l^{(j)} - 1 \qquad (i = 1, \ldots, j-1),\ (j = 2, \ldots, k-1), \\ &\beta_i^{(j)} := \textstyle\sum_{l=1}^{i}\mu_l^{(j)} - 1 \qquad (i = 1, \ldots, k-1),\ (j = k, k+1, \ldots). \end{aligned} \tag{2.10}$$

It turns out that the k-step parameters $\{\mu_i^{(j)}\}_{i=0}^{k}$ have limits as $j \to \infty$, i.e.,

$$\mu_i := \lim_{j\to\infty}\mu_i^{(j)} \quad (i = 0, 1, \ldots, k).$$

To show this, it is known (cf. Curtiss [2, p. 584]) that

$$\lim_{m\to\infty}\frac{F_{m-1}}{F_m}\frac{(z)}{(z)} = \frac{1}{\Phi_k(z)} \qquad (\text{for any } z \in \mathbb{C}\backslash\Omega_k(\rho_0)).$$

Here, $w = \Phi_k(z)$ denotes the *inverse mapping* of Ψ_k, i.e., Φ_k conformally maps $\bar{\mathbb{C}}\backslash\Omega_k(\rho_0))$ onto $\bar{\mathbb{C}}\backslash\{|w| \le 1\}$. Since $0 \notin \Omega_k(\rho_0)$ by hypothesis and $\Psi_k(w_0) = 0$, then $w_0 = \Phi_k(0)$. Hence, it follows from (2.7) and the above display (with $z = 0$) that

$$\mu_0 := -\frac{1}{cw_0},\ \mu_i := -\frac{c_{i-1}}{c(w_0)^i} \quad (i = 1, \ldots, k); \tag{2.11}$$

This means that the k-step iteration, generated by Faber polynomials, asymptotically becomes a *stationary method*, and it is the convergence of this stationary limit that we will actually optimize in what is to follow. Alternatively, one could also perform, from the first vector iteration, a stationary k-step method based on the converged coefficients $\{\mu_i\}_{i=0}^{k}$ of (2.11) and the associated recurrence relations of (2.6). More will be said about the relationship between the iteration (2.6) and stationary k-step methods below.

Let us briefly consider the special case $k = 2$. The conformal mapping function is then given by

$$\Psi_2(w) = cw + c_0 + \frac{c_1}{w} \quad (c \ne 0 \text{ and } c_1 \ne 0)\,. \tag{2.12}$$

Consider the equation

$$\Psi_2'(w) = c - \frac{c_1}{w^2} = 0\,, \tag{2.13}$$

which yields $\rho_0 = \sqrt{|c_1|/|c|}$. In this case, $\partial\Omega_2(\rho_0)$ is a line segment with end points $c_0 \pm 2\sqrt{cc_1}$, which are either both real or a complex conjugate pair. Thus, $\Psi(w)$ maps the exterior of the disk $\{w \in \mathbb{C} : |w| \le \rho_0\}$ conformally onto the exterior of a line segment.

Using (2.6), we obtain the formulas for the associated two-step iteration,

$$\begin{aligned} \mathbf{x}_1 &= \mu_0^{(1)}\mathbf{r}_0 + \mathbf{x}_0 , \\ \mathbf{x}_j &= \mu_0^{(j)}\mathbf{r}_{j-1} + \mu_1^{(j)}\mathbf{x}_{j-1} + \mu_2^{(j)}\mathbf{x}_{j-2} \quad (j = 2, 3, \ldots), \end{aligned} \tag{2.14}$$

where

$$\mu_0^{(1)} = \frac{1}{c_0} , \; \mu_0^{(j)} = -\frac{1}{c}\frac{F_{j-1}(0)}{F_j(0)} \quad (j = 2, 3, \ldots),$$

$$\mu_1^{(j)} = -\frac{c_0}{c}\frac{F_{j-1}(0)}{F_j(0)} \quad (j = 2, 3, \ldots),$$

$$\mu_2^{(2)} = -2\frac{c_1}{c}\frac{1}{F_2(0)} , \; \mu_2^{(j)} = -\frac{c_1}{c}\frac{F_{j-2}(0)}{F_j(0)} \quad (j = 3, 4, \ldots).$$

The iteration parameters can be updated using (2.2), which leads to

$$\mu_0^{(2)} = \frac{c_0}{c_0^2 - 2c^2} , \; \mu_1^{(2)} = c_0\mu_0^{(2)} , \; \mu_2^{(2)} = \frac{2cc_1}{c_0^2 - 2c^2} ,$$

and, for $j = 3, 4, \ldots$,

$$\mu_0^{(j)} = \frac{1}{c_0 - cc_1\mu_0^{(j-1)}} , \; \mu_1^{(j)} = c_0\mu_0^{(j)} , \; \mu_2^{(j)} = \left[1 - \frac{c_0}{cc_1\mu_0^{(j-1)}}\right]^{-1} .$$

This is exactly the well-known recurrence relation for the parameters of the (two-step) Chebyshev iteration (cf. [11, Sect. 2.5]).

Returning to the general k-step method, for each complex number ζ in the z-plane, define the function $R(\zeta)$ by

$$R(\zeta) := \begin{cases} \rho_0, \text{ if } \zeta \in \Omega_k(\rho_0), \\ \min\{\rho : \rho \ge \rho_0 \text{ and } \zeta \in \Omega_k(\rho). \end{cases}$$

With the assumption that $0 \notin \Omega_k(\rho_0)$, the asymptotic convergence factor associated with a k-step method generated by (2.1), for a given set of parameters, $c, c_0, \ldots, c_{k-1}$, is given by

$$\overline{\lim_{j\to\infty}} \left[\sup_{\mathbf{e}_0 \neq 0} \frac{\|\mathbf{e}_j\|}{\|\mathbf{e}_0\|}\right]^{1/j} \le \max_{\zeta\in\sigma(A)} \left\{\frac{R(\zeta)}{|w_0|}\right\} =: \gamma_k(c, c_0, \ldots, c_{k-1}; \sigma(A)) , \tag{2.15}$$

where $\mathbf{e}_j := \mathbf{x} - \mathbf{x}_j$ is the error at step j and $\sigma(A)$ denotes the spectrum of the matrix A of (1.1) (cf. Niethammer and Varga [16, Sect. 4] and Eiermann [3, Sect. 2]). This leads to the problem of choosing $c, c_0, \ldots, c_{k-1}$ to minimize $\gamma_k(c, c_0, \ldots, c_{k-1}; \sigma(A))$. We denote the associated infimum by

$$\Gamma_k(\sigma(A)) := \inf_{c, c_0, \ldots, c_{k-1}} \gamma_k(c, c_0, \ldots, c_{k-1}; \sigma(A)). \tag{2.16}$$

For all practical purposes, the spectrum $\sigma(A)$ is certainly not known, but some information about the spectrum is usually known, as will be described below. So, we now assume that $\{\zeta_i\}_{i=1}^p$ are given nonzero points in the complex plane, consisting of real points or conjugate complex pairs of points (because A is a real square matrix), which gives information about the spectrum of A. Based only on this limited information, the problem of (2.16) is then *modified* to determining (or approximating) the parameters $c, c_0, \ldots, c_{k-1}$ that yield the associated infimum,

$$\Gamma_k(\{\zeta_i\}_{i=1}^p) := \inf_{c, c_0, \ldots, c_{k-1}} \gamma_k(c, c_0, \ldots, c_{k-1}; \{\zeta_i\}_{i=1}^p) . \tag{2.17}$$

To determine the quantity in (2.17), we must, from (2.15), evaluate the number $R(\zeta_i)$. Consider the equation

$$\Psi_k(w) = cw + c_0 + \frac{c_1}{w} + \ldots + \frac{c_{k-1}}{w^{k-1}} = \zeta_i. \tag{2.18}$$

This equation has k roots, which are the roots of the associated polynomial

$$cw^k + (c_0 - \zeta_i)w^{k-1} + \ldots + c_{k-2}w + c_{k-1} = 0. \tag{2.19}$$

We denote these roots by $\omega_i^{(j)}$, for $j = 1, \ldots, k$. If $\zeta_i \notin \Omega_k(\rho_0)$, then one and only one of the roots, say $\omega_i^{(1)}$, will satisfy $|\omega_i^{(1)}| > \rho_0$. This follows because $\Psi_k(w)$ is a conformal mapping from the exterior of $\{w \in \mathbb{C} : |w| \leq \rho_0\}$ onto the exterior of $\Omega_k(\rho_0)$. If $\zeta_i \in \Omega_k(\rho_0)$, then $|\omega_i^{(j)}| \leq \rho_0$ for $j = 1, \ldots, k$. Thus, in either case, we may define

$$R(\zeta_i) := \max\{\rho_0, |\omega_i^{(1)}|, \ldots, |\omega_i^{(k)}|\}. \tag{2.20}$$

We now offer a *geometrical picture* for the convergence factor $\gamma_k(c, c_0, \ldots, c_{k-1}; \{\zeta_i\}_{i=1}^p)$ in (2.17). Given the parameters $c, c_0, \ldots, c_{k-1}$, assume that $0 \notin \Omega_k(\rho_0)$. Let $\hat{\rho} \geq \rho_0$ be the smallest value such that $\{\zeta_i\}_{i=1}^p \subset \Omega_k(\hat{\rho})$. Likewise, let $\hat{\rho}_0$ be the smallest value such that $0 \in \Omega_k(\hat{\rho}_0)$. Then, it follows that

$$\gamma_k(c, c_0, \ldots, c_{k-1}; \{\zeta_i\}_{i=1}^p) = \frac{\hat{\rho}}{\hat{\rho}_0}\ . \tag{2.21}$$

It is important to mention, given any nonzero points $\{\zeta_i\}_{i=1}^p$ which consist of either real or complex conjugate pairs of points, that

i) $\Gamma_k(\{\zeta_i\}_{i=1}^p) = 1$ *can* occur for certain values of k, and
ii) $\Gamma_k(\{\zeta_i\}_{i=1}^p) < 1$ for *all* k sufficiently large if and only if the *real* points of $\{\zeta_i\}_{i=1}^p$ are all of the same sign.

The first statement, i), can occur, for example, if the nonzero numbers $\{\zeta_i\}_{i=1}^4$ are chosen to be the fourth roots of -1 and if $k = 1$. In this case, $\Psi_1(w) = cw + c_0, \Phi_1(z) = (z - c_0)/c$, and $\Omega_1(\rho)$ is a disk with center c_0 and radius $|\rho c|$. It is geometrically clear in this case that $\{\zeta_i\}_{i=1}^4 \subset \Omega_1(\rho)$ if and only if $0 \in \Omega_1(\rho)$, which implies that $\gamma_1(c, c_0; \{\zeta_i\}_{i=1}^p) > 1$, with $\gamma_1(c, c_0; \{\zeta_i\}_{i=1}^p) \to 1$ as $c_0 \to \infty$. This first statement, i), is also shown to be the case in Table 5.1 for Example 5.1 when $k = 1$ or $k = 2$. The second statement, ii), is a theoretical result which is a consequence of the construction in [21] where the Schwarz-Christoffel mapping of polygonal domains is used. (The details for this will be given elsewhere.)

Now, the relation between a *stationary* k-step iteration and the minimization problem (2.17) can also be established without any assumption on the conformality of Ψ_k. In order to do this, we may assume, with the stationary values of (2.11), that $\mu_k \neq 0$ (since from (2.6), we would otherwise have a stationary $(k-1)$-step method), and we write the k-step iterations as

$$\begin{bmatrix} \mathbf{r}_{j-k+1} \\ \vdots \\ \mathbf{r}_{j-1} \\ \mathbf{r}_j \end{bmatrix} = \begin{bmatrix} O & I & & \\ \vdots & \ddots & \ddots & \\ O & \ldots & O & I \\ \mu_k I & \ldots & \mu_2 I & \mu_1 I - \mu_0 A \end{bmatrix} \begin{bmatrix} \mathbf{r}_{j-k} \\ \vdots \\ \mathbf{r}_{j-2} \\ \mathbf{r}_{j-1} \end{bmatrix} \tag{2.22}$$

(cf. [13]). Calling C_k the block-companion matrix in (2.22) and assuming also that $\mu_0 \neq 0$ (so that C_k is actually dependent on A), it can be verified that $\tau \in \sigma(C_k)$ if and only if τ is a (nonzero) solution of

$$\tau^k - (\mu_1 - \mu_0\zeta_i)\tau^{k-1} - \mu_2\tau^{k-2} - \ldots - \mu_k = 0, \tag{2.23}$$

where $\zeta_i \in \sigma(A)$, and where we denote these zeros of (2.23) by $\tau_i^{(j)}$ for $j = 1, \ldots, k$. In the context of the conformal mapping Φ_k and on using (2.11), this yields

$$c(\tau_i^{(j)}\omega_0) + c_0 + \frac{c_1}{\tau_i^{(j)}\omega_0} + \cdots + \frac{c_{k-1}}{(\tau_i^{(j)}\omega_0)^{k-1}} = \zeta_i\ .$$

¿From (2.18) and (2.20) we see that $\tau_i^{(j)} = \omega_i^{(j)}/\omega_0$, and thus, $|\tau_i^{(j)}| \leq R(\zeta_i)/|\omega_0|$. Equation (2.11) implies a one-to-one correspondence between the parameters $c, c_0, \ldots, c_{k-1}$ with $c \neq 0$ and $\mu_0, \mu_1, \ldots, \mu_k$, with $\sum_{i=1}^k \mu_i = 1$. Therefore, minimizing the spectral radius of the matrix C_k of (2.22) leads to

$$\inf_{\substack{\mu_0, \mu_1, \ldots, \mu_k \\ \mu_1 + \cdots + \mu_k = 1}} \{ \max_{\substack{1 \leq i \leq p \\ 1 \leq j \leq k}} |\tau_i^{(j)}| \} \leq \inf_{\substack{c, c_0, c_1, \ldots, c_k \\ c \neq 0}} \{ \max_{1 \leq i \leq p} \frac{R(\zeta_i)}{|\omega_0|} \} = \Gamma_k(\{\zeta_i\}_{i=1}^p),$$

the last equality following from (2.17). The stationary k-step method involves essentially the same min-max problem as the nonstationary method (2.6). It can be shown that for the optimal choice of parameters, there will always be an active constraint and thus the two methods will have the same asymptotic convergence factor.

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Sets of points $\{\zeta_1, \ldots, \zeta_p\}$ that approximate $\sigma(A)$ can be obtained from applying Arnoldi's method, which computes an orthogonal projection of the matrix $A \in \mathbb{R}^{N\times N}$ onto the Krylov subspace

$$\mathcal{K}_n(\mathbf{r}_0, A) := \operatorname{span}\{\mathbf{r}_0, A\mathbf{r}_0, \ldots, A^{n-1}\mathbf{r}_0\} .$$

Arnoldi's method specifically computes an orthonormal basis for $\mathcal{K}_n(\mathbf{r}_0, A)$, using a modified Gram-Schmidt procedure. If the columns of $V_n \in \mathbb{R}^{N\times n}$ contain these basis vectors, the upper Hessenberg matrix $H_n = V_n^T A V_n \in \mathbb{R}^{n\times n}$ comes out as a by-product from the Arnoldi procedure (see Saad [18, Chapter VI] for details). The n eigenvalues of H_n, the so-called Rayleigh-Ritz values of A, often approximate quite well the spectrum, $\sigma(A)$ of A. These points are therefore commonly used as a starting point upon which a polynomial iteration can be based.

3. Algorithms for the Computation of k-Step Iteration Parameters. Given the $k+1$ real parameters $c \neq 0, c_0, \ldots, c_{k-1}$, assume that $0 \notin \Omega_k(\rho_0)$. We will show below that this is easy to accomplish. As before, we define ω_0 to be the unique root of largest modulus of

$$cw + c_0 + \frac{c_1}{w} + \cdots + \frac{c_{k-1}}{w^{k-1}} = 0 ,$$

or equivalently, ω_0 is the unique zero of largest modulus of the associated polynomial

$$cw^k + c_0 w^{k-1} + \cdots + c_{k-1} = 0 .$$

Given the set $\{\zeta_i\}_{i=1}^p$, let S be the smallest number $S \geq \rho_0$ such that $\{\zeta_i\}_{i=1}^p \subset \Omega_k(S)$. Let ω_j be any zero of largest modulus of

$$cw + c_0 + \frac{c_1}{w} + \cdots + \frac{c_{k-1}}{w^{k-1}} = \zeta_j \ (j = 1, 2, \cdots, p) , \tag{3.1}$$

so that the constraints $\{\zeta_i\}_{i=1}^p \subset \Omega_k(S)$ imply that $|\omega_j| \leq S$ for $j = 1, \ldots, p$. A straightforward way to compute the solution of (2.17) is then to solve

$$\min_{c, c_0, c_1, \ldots, c_{k-1} \in \S} \frac{S}{|\omega_0|}, \tag{3.2}$$

under the constraints $|\omega_j| \leq S$ for $j = 1, \ldots, p$. This is equivalent to

$$\min_{c, c_0, c_1, \ldots, c_{k-1} \in \S} -\ln\left(\frac{|\omega_0|}{S}\right), \tag{3.3}$$

under the constraints $\ln(|\omega_j|/S) \leq 0$ for $j = 1, \ldots, p$. In the language of nonlinear programming, this means that our aim is the minimization of the objective function

$$J(c, c_0, \ldots, c_{k-1}) := -\ln\left(\frac{|\omega_0|}{S}\right),$$

subject to the constraints $\nu_j(c, c_0, \ldots, c_{k-1}) \leq 0$ with

$$\nu_j(c, c_0, \ldots, c_{k-1}) := \ln\left(\frac{|\omega_j|}{S}\right) , \ (j = 1, \ldots, p) .$$

In the form of (3.3), we can directly apply the Kuhn-Tucker conditions (see Ciarlet [1, Theorem 9.2-3]) which give necessary conditions for a minimum. These conditions state that there exist multipliers $\eta_j \geq 0$ such that

$$\frac{\partial}{\partial c} J(c, c_0, \ldots, c_{k-1}) + \sum_{j=1}^{p} \eta_j \frac{\partial}{\partial c} \nu_j(c, c_0, \ldots, c_{k-1}) = 0 ,$$

$$\frac{\partial}{\partial c_i} J(c, c_0, \ldots, c_{k-1}) + \sum_{j=1}^{p} \eta_j \frac{\partial}{\partial c_i} \nu_j(c, c_0, \ldots, c_{k-1}) = 0 \quad (i = 0, 1, \cdots, k-1),$$

where $\eta_j = 0$ if the corresponding constraint is not active, i.e., when $\nu_j(c, c_0, \ldots, c_{k-1}) < 0$. Applied to (3.3), this leads to

$$\frac{1}{\omega^i \Psi_k'(\omega_0)} = \sum_{j=1}^{p} \frac{\eta_j}{\omega_j^i \Psi_k'(\omega_j)}$$

for $i = 0, 1, \ldots, k-1, k$ where $\eta_j = 0$ if $|\omega_j| < S$ and $\eta_j \geq 0$ if $|\omega_j| = S$. Efficient algorithms for the solution of such constrained optimization problems make use of the gradients of the objective as well as the constraint functions (cf. Gill et al. [6, Ch. 6]).

We have to make sure that our starting guess satisfies $0 \notin \Omega_k(\rho_0)$ and that this condition is maintained in the course of the optimization procedure. This can be implemented as an additional constraint in the optimization problem. As an initial guess for the k-step parameters $c, c_0, c_1, \ldots, c_{k-1}$ for starting the optimization procedure, one can choose, for example, $c_1 = \cdots = c_{k-1} = 0$ and $c, c_0 \neq 0$. This is equivalent to a one-step method, and the condition $0 \notin \Omega_k(\rho_0)$ is trivially fulfilled since $\Omega_k(\rho_0) = \{c_0\}$ with $\rho_0 = 0$. In practice, it is more appropriate to use the optimal $(k-1)$-step parameters, with $c_{k-1} = 0$, as a starting guess for the optimization routine for the k-step parameters.

Again, in practice, we are not necessarily interested in exactly solving the above min-max problem. Instead, we are satisfied with parameters which only *nearly* minimize (2.17) if these parameters can be obtained with less expense. For some $q \in \mathbf{N}$, let us consider

$$\min_{c, c_0, c_1, \ldots, c_{k-1}} \frac{1}{|\omega_0|} \left(\sum_{j=1}^{p} |\omega_j|^{2q} \right)^{1/2q} =: \frac{1}{|\tilde{\omega}_0|} \left(\sum_{j=1}^{p} |\tilde{\omega}_j|^{2q} \right)^{1/2q} . \tag{3.4}$$

For the solution of this problem, we obtain

$$\frac{1}{|\tilde{\omega}_0|} \max_{1 \leq j \leq p} |\tilde{\omega}_j| \leq \frac{1}{|\tilde{\omega}_0|} \left(\sum_{j=1}^{p} |\tilde{\omega}_j|^{2q} \right)^{1/2q} \leq p^{1/2q} \min_{c, c_0, c_1, \ldots, c_{k-1}} \frac{1}{|\omega_0|} \max_{1 \leq j \leq p} |\omega_j| , \tag{3.5}$$

i.e., for sufficiently large q, the solution of (3.4) will be close to optimal for the original minimization problem (2.17). In actual computations, these two problems will be much more closely connected than the above estimate predicts. We will see in Section 5 that the solution of (3.4) already leads to useful k-step parameters for moderate values of q.

We close this section with some remarks on the numerical solution of (3.4). First, we are free to choose $\tilde{\omega}_0 = 1$ which leads to $\Psi_k(1) = c + c_0 + \cdots + c_{k-1} = 0$, eliminating one of the parameters, say, c. From this, we are led to the *unconstrained* minimization problem

$$\min_{c_0, c_1, \ldots, c_{k-1}} \sum_{j=1}^{p} |\omega_j|^{2q} \tag{3.6}$$

which we can again solve using the gradients

$$\frac{\partial}{\partial c_i} \sum_{j=1}^{p} |\omega_j|^{2q} = \sum_{j=1}^{p} |\omega_j|^{2q} \mathrm{Re} \left[\left(1 - \frac{1}{\omega_j^{i+1}} \right) \frac{1}{\Psi_k'(\omega_j)} \right] \quad (i = 0, 1, \cdots, k-1).$$

The application of standard minimization routines to this formulation usually yields a solution after a small number of iterative steps. In each step, the computation of $\omega_j, 1 \leq j \leq p$ amounts to finding a root of largest modulus of a polynomial of degree k. Clearly, the solution of such an unconstrained optimization problem for a differentiable function is much less expensive than the constrained optimization problem associated with (3.3). In our computational experiments, to be presented in Section 5, we used the MATLAB optimization toolbox. The procedures for unconstrained, as well as for constrained, optimization make use of gradients by means of a quasi-Newton scheme as described in [6, Ch. 6].

4. Strategies for the Adaptive Implementation. In this section, we generalize certain techniques, developed in [12] for $k = 2$, to the case of general k-step methods. Let us suppose that the iteration was initiated with some choice of parameters $c, c_0, \ldots, c_{k-1}$, based on a priori knowledge of $\sigma(A)$, perhaps from a hybrid strategy involving a GMRES iteration. The adaptive strategy will be based on new information which is collected while carrying out the k-step method. After a certain number of iterations, say n_0, we begin computing an orthogonal basis of the space spanned by the consecutive residuals $\mathbf{r}_{n_0}, \ldots, \mathbf{r}_{n_0+n-1}$. Again, this can be accomplished by a modified Gram-Schmidt process, i.e., on starting with $\mathbf{w}_1 = \mathbf{r}_{n_0}/\beta$ with $\beta := \|\mathbf{r}_{n_0}\|_2$ for $j = 1, 2, \ldots, n$, we compute

$$\left\{ \begin{array}{l} \hat{\mathbf{w}}_{j+1} = \mathbf{r}_{n_0+j} , \\ \hat{h}_{i,j} = \mathbf{w}_i^T \hat{\mathbf{w}}_{j+1} , \ \hat{\mathbf{w}}_{j+1} = \hat{\mathbf{w}}_{j+1} - \hat{h}_{i,j} \mathbf{w}_i , \ i = 1, \ldots, j , \\ \hat{h}_{j+1,j} = \|\hat{\mathbf{w}}_{j+1}\|_2 , \ \mathbf{w}_{j+1} = \hat{\mathbf{w}}_{j+1} / \hat{h}_{j+1,j} . \end{array} \right. \tag{4.1}$$

The matrix $W_n = [\mathbf{w}_1, \ldots, \mathbf{w}_n]$ contains an orthonormal basis for the subspace spanned by $\mathbf{r}_{n_0}, \ldots, \mathbf{r}_{n_0+n-1}$. The residual $\mathbf{r}_{n_0}$ can be expected to be a pre-filtered residual, i.e., a vector rich in just a few eigenvector components corresponding to dominant eigenvalues of the k-step iteration operator. Thus, the vectors $\mathbf{r}_{n_0}, \ldots, \mathbf{r}_{n_0+n-1}$ may be nearly linearly dependent. Numerical difficulties can be avoided by applying a rank-revealing variation of the modified Gram-Schmidt process to the least-squares problem

$$\min_{\pi_0,\ldots,\pi_{n-1}} \|\mathbf{r}_{n_0} + \sum_{k=1}^{n} \pi_k \mathbf{r}_{n_0+k}\|_2 \,. \tag{4.2}$$

If the scalar $\hat{h}_{j+1,j}$ in (4.1) becomes small relative to $\left(\sum_{k=1}^{j+1} \hat{h}_{k,j}^2\right)^{1/2} = \|\hat{\mathbf{w}}_{j+1}\|_2$, then problem (4.2) is nearly consistent and should be restricted to $n = j$.

The roots of the polynomial equation

$$\tau^n + \pi_{n-1}\tau^{n-1} + \cdots + \pi_1\tau + \pi_0 = 0$$

then coincide with the eigenvalues of the Hessenberg matrix $\hat{H}_n$ due to the equivalence of the (modified) Arnoldi process and the polynomial minimization problem (4.2) (cf. Saad [18, Theorem 6.1 and remarks thereafter]). It should also be mentioned that this least-squares algorithm is exactly what was called the "modified power method" in [12].

As pointed out in Section 2, the k-step parameters tend to the stationary values

$$\mu_0 = -\frac{1}{c\omega_0}\,,\; \mu_i = -\frac{c_{i-1}}{c(\omega_0)^i} \;\; (i = 1, \ldots, k)\,.$$

If we again use the normalization $c + c_0 + c_1 + \cdots + c_{k-1} = 0$, i.e., $\omega_0 = 1$, then

$$\mu_0 = -\frac{1}{c}\,,\; \mu_i = -\frac{c_{i-1}}{c} \;\; (i = 1, \ldots, k)\,.$$

In order to set up a connection between the orthogonal section of the iteration operator and the orthogonal section for A, it is convenient to recall from (2.22) that

$$\begin{bmatrix} \mathbf{r}_{j-k+1} \\ \vdots \\ \mathbf{r}_{j-1} \\ \mathbf{r}_j \end{bmatrix} = \begin{bmatrix} O & I & & \\ \vdots & \ddots & \ddots & \\ O & \cdots & O & I \\ \mu_k I & \cdots & \mu_2 I & \mu_1 I - \mu_0 A \end{bmatrix} \begin{bmatrix} \mathbf{r}_{j-k} \\ \vdots \\ \mathbf{r}_{j-2} \\ \mathbf{r}_{j-1} \end{bmatrix},$$

and that therefore the eigenvalues of the block companion matrix C_k determine the convergence rate of the k-step method. The eigenvalues of $\hat{H}_n$ may be viewed as approximations to the extreme eigenvalues of this companion matrix.

As stated above, for $\mu_0 \neq 0$, if $\lambda \in \sigma(A)$, then each solution of

$$\tau^k - (\mu_1 - \mu_0\lambda)\tau^{k-1} - \mu_2\tau^{k-2} - \cdots - \mu_k = 0$$

is an eigenvalue of C_k in (2.22). Conversely, if $\tau \in \sigma(C_k)$, then

$$\lambda = -\frac{1}{\mu_0}\left[\tau - \mu_1 - \frac{\mu_2}{\tau} - \cdots - \frac{\mu_k}{\tau^{k-1}}\right] = c\tau + c_0 + \frac{c_1}{\tau} + \cdots + \frac{c_{k-1}}{\tau^{k-1}}$$

is an eigenvalue of A. This implies that an eigenvalue estimate $\hat{\tau} \in \sigma(\hat{H}_n)$ for the k-step iteration operator leads to an eigenvalue estimate

$$\hat{\lambda} = -\frac{1}{\mu_0}\left[\hat{\tau} - \mu_1 - \frac{\mu_2}{\hat{\tau}} - \cdots - \frac{\mu_k}{\hat{\tau}^{k-1}}\right] = c\hat{\tau} + c_0 + \frac{c_1}{\hat{\tau}} + \cdots + \frac{c_{k-1}}{\hat{\tau}^{k-1}}$$

for the matrix A.

Using this technique, new points $\hat{\zeta}_1, \ldots, \hat{\zeta}_{\hat{p}}$ are obtained which give new information on the spectrum of A, and these new points can be used to *modify* our existing k-step method. In analogy with the procedure described in [12, Section 6], we *merge* these newly obtained eigenvalue estimates with those of the previous set of points $\zeta_1, \ldots, \zeta_p$ that determined the initial near-optimal k-step method. This merging avoids discarding useful previous information on the location of $\sigma(A)$.

Finally, we would like to point out that we will not always recommend using the above adaptive procedure. Instead, one compares the *observed* convergence behavior of the existing k-step method with its *predicted* convergence factor. If the iteration is converging as predicted, or nearly so, then there is no need to find new parameters. If the convergence is significantly slower than predicted, then one of two adaptive procedures is recommended. If the iteration parameters $\mu_i^{(j)}$ have reached their limit values μ_i as in (2.11), the method described above should be used. If the limit values have not been reached, then a hybrid method that employs a fixed number of GMRES steps should be implemented and the Arnoldi roots used as new eigenvalue estimates.

5. Computational Experiments. We will now illustrate the convergence behavior of our adaptive k-step algorithm in two examples.

EXAMPLE 5.1. We start with a normal matrix A in $\mathbb{R}^{256\times 256}$ with eigenvalues uniformly distributed in the half-annulus

$$\{z \in \mathbb{C} : 0.5 \leq |z| \leq 1 \,,\ \mathrm{Re} z \geq 0\}$$

(cf. [14, Example 1]). At first, we compute the near-optimal k-step methods ($1 \leq k \leq 8$), for various values of q, with respect to the *exact* spectrum of A. The corresponding convergence factors (i.e., estimates of $\gamma_k(c, c_0, \ldots, c_{k-1}; \sigma(A)$ of (2.15)) are shown in Table 5.1. Since some of the eigenvalues of A are located on the imaginary axis, (cf. Fig. 5.1), the 1- and 2-step methods will not converge here. This example shows that higher-degree k-step methods are convergent in cases where the Chebyshev (2-step) method cannot converge, since there is no circle or ellipse that separates the spectrum from the origin. Clearly, if we solve the minimization problem (2.16) exactly ($q = \infty$), the associated convergence factors are nonincreasing as k increases. Apparently, this is not always true for finite q, as Table 5.1 shows.

TABLE 5.1
k-step convergence factors for Example 5.1 with respect to exact eigenvalues

k	$q=1$	$q=2$	$q=3$	$q=4$	$q=\infty$
1	—	—	—	—	—
2	—	—	—	—	—
3	—	—	0.9996	0.9997	0.9995
4	—	0.9933	0.9834	0.9857	0.9736
5	—	0.9828	0.9784	0.9782	0.9645
6	0.9986	0.9893	0.9763	0.9762	0.9567
7	0.9889	0.9792	0.9828	0.9786	0.9481
8	0.9810	0.9735	0.9702	0.9673	0.9383

In order to choose the optimal k, we compute the "cost factors"

$$f_k(q) := -(\varepsilon + k)\lceil \frac{1}{\log \kappa_k(q)} \rceil \,. \tag{5.1}$$

In (5.1) and in the sequel, $\kappa_k(q)$ always denotes the first term in (3.5) , i.e.,

$$\kappa_k(q) := \frac{1}{|\tilde{\omega}_0|} \max_{1\leq j\leq p} |\tilde{\omega}_j|,$$

which is the convergence factor, measured in the maximum norm, associated with the optimal parameters with respect to the l^{2q}-norm. If ε denotes the average number of non-zero elements per row in the matrix A, then $\kappa_k(q)$ is the number of vector operations "expected" to be carried out in order to reduce the error by a factor of 10. For example, we chose $\varepsilon = 5$, in (5.1), though it should be noted that a more realistic cost factor should also depend on the particular machine used. The results are given in Table 5.2.

TABLE 5.2
k-step cost factors for Example 5.1 with respect to exact eigenvalues

k	$q=1$	$q=2$	$q=3$	$q=4$	$q=\infty$
1	∞	∞	∞	∞	∞
2	∞	∞	∞	∞	∞
3	∞	∞	4168	61168	37552
4	∞	3078	1242	1449	783
5	∞	1330	1060	1050	640
6	17523	2354	1067	1056	572
7	2496	1320	1596	1284	528
8	1560	1118	1001	910	481

It is of interest to point out that, because the half-annulus of Example 5.1 is a compact set which excludes the origin, there is a unique $\Phi(z)$ which conformally maps the exterior of the half-annulus onto $\{w \in \mathbb{C} : |w| > 1\}$, with $\Phi(\infty) = \infty, \Phi'(\infty) > 0$, and $|\Phi(0)| = |\omega_0| > 1$. (We note that because of the corners of the half-annulus, the inverse mapping of $\Phi(z)$, namely $\Psi(w)$, cannot be of the form (2.1) for any $k \in \mathbb{N}$.) By definition, we have

$$\kappa_k(\infty) \geq \kappa_{k+1}(\infty) \geq \cdots \geq \frac{1}{|\omega_0|}, \text{ with } \lim_{k\to\infty} \kappa_k(\infty) = \frac{1}{|\omega_0|}.$$

Hence, on writing

$$\frac{-1}{\log \kappa_k(\infty)} =: \frac{1}{\log |\omega_0|} + \epsilon_k, \text{ where } \epsilon_k \geq \epsilon_{k+1} \text{ for all } k \text{ and } \lim_{k\to\infty} \epsilon_k = 0,$$

it follows that the cost factors $f_k(\infty)$ can be expressed as

$$f_k(\infty) = (\epsilon + k)\left\{\frac{-1}{\log \kappa_k(\infty)}\right\} = \frac{k}{\log |\omega_0|} + k\delta_k + \frac{\epsilon}{\log |\omega_0|} + \epsilon\delta_k \, .$$

But this shows that these cost factors grow at least *linearly* in k as $k \to \infty$, and are consequently, *unbounded* as $k \to \infty$. Hence, there always exists a least $k \in \mathbb{N}$ which minimizes these cost factors (for $q = \infty$). The final column of Table 5.4 indicates this, and this is the main reason *why* optimized k-step methods are attractive in practical situations.

In practice, the construction of k-step parameters has to be based on estimates of the eigenvalues of A, rather than on exact eigenvalues of A. We applied our k-step algorithm to the 16 Rayleigh-Ritz values obtained from the Arnoldi process, and these Rayleigh-Ritz values are indicated by asterisks in Figure 5.1. Also shown in Figure 5.1 are the level curves

$$\partial\Omega_k(\rho) = \{z = \Psi_4(w) : |w| = \rho\}$$

for $\rho = \kappa$ (the associated convergence factor) and $\rho = 1$ for a 4-step method with $q = 4$, constructed by the above procedure. The fact that the entire spectrum is contained inside the level curve corresponding to $\rho = 1$ implies that this 4-step method will converge.

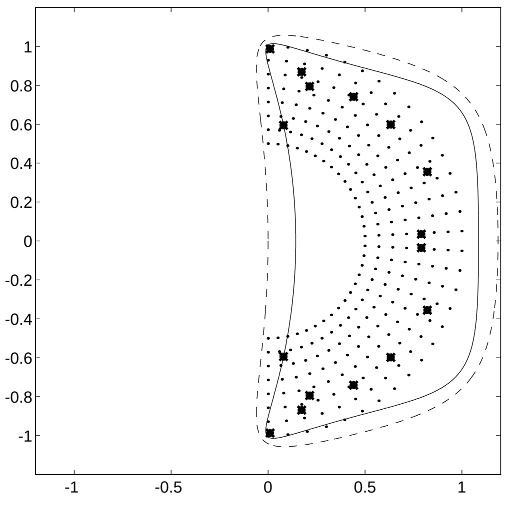

FIG. 5.1. *4-step level lines Example 5.1*

EXAMPLE 5.2. This example is very similar to that of [21, Example 6.2], and arises from the discretization of the elliptic boundary value problem,

$$\begin{aligned} -\Delta u + \mu u_x &= f\,, \quad (x,y) \in U = (0,1)\times(0,1)\,, \\ u(x,y) &= 0\,, \quad (x,y) \in \partial U\,, \end{aligned} \tag{5.2}$$

by central differences. We solve this boundary value problem on a grid with 32 interior points in each direction, leading to a linear system of dimension 1024. Moreover, we chose μ in such a way that $\mu h/2$, the associated grid Reynolds number, equals 2. In practice, one would, of course,

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not apply an iterative scheme directly to this linear system but to a suitably preconditioned one. Since our goal is to investigate the underlying basic iterative process and since we want to keep our results transparent, we use the non-preconditioned linear system as our example. We would expect, however, the same qualitative results from investigating a preconditioned problem and, of course, from problems of larger size.

Table 5.3
k-step convergence factors for Example 5.2 with respect to exact eigenvalues

k	$q=1$	$q=2$	$q=3$	$q=4$	$q=\infty$
1	0.8669	0.8674	0.8681	0.8682	0.8639
2	0.8327	0.8201	0.8099	0.8030	0.7812
3	0.8294	0.8052	0.7886	0.7786	0.7488
4	0.8134	0.7659	0.7335	0.7149	0.6976
5	0.7992	0.7265	0.7259	0.7223	0.6950
6	0.7928	0.7356	0.7340	0.7306	0.6876
7	0.7658	0.7424	0.7419	0.7408	0.6870
8	0.7398	0.7434	0.7464	0.7444	0.6863

Table 5.4
k-step cost factors for Example 5.2 with respect to exact eigenvalues

k	$q=1$	$q=2$	$q=3$	$q=4$	$q=\infty$
1	96	96	96	96	96
2	91	84	77	77	70
3	104	88	80	80	64
4	108	81	72	63	63
5	110	80	80	80	70
6	110	88	88	88	77
7	108	96	96	96	84
8	104	104	104	104	91

Interestingly, Table 5.4 shows that the optimal k with respect to the estimated cost factor for the exact eigenvalues is reached here at a relatively low degree, namely $k = 4$. When we start with a random right hand side $\mathbf{b}$ and zero initial guess $\mathbf{x}_0$, we see in Table 5.5 that, with respect to the Rayleigh-Ritz values obtained after 16 Arnoldi steps, the lowest cost factor is again obtained for the 4-step method, with $q = 4$.

Table 5.5
k-step convergence and cost factors for Example 5.2, with respect to 16 Rayleigh-Ritz values, and a random right hand side

k	κ	cost factor
1	0.8936	126
2	0.8680	119
3	0.8541	120
4	0.8138	108
5	0.8191	120
6	0.8185	132
7	0.8203	144
8	0.8107	143

In Figure 5.2 we can see that the spectrum of the associated matrix is well captured by the level curve with $\rho = \kappa$, corresponding to the optimal 4-step method with $q = 4$. Indeed, Figure 5.3 shows that the actual convergence of this 4-step method (solid line) is fast and smooth.

For comparison, we also include, in Figure 5.3, GMRES(16), the restarted version of GMRES [19] (dashed line), the hybrid GMRES algorithm by Nachtigal, Reichel and Trefethen [15] (dash-dotted line), and transpose-free QMR method of Freund [5] (dotted line). The hybrid GMRES algorithm uses the residual polynomial obtained after 16 steps of GMRES and performs the corresponding iteration repeatedly by means of Richardson iteration. For the transpose-free QMR method, both starting

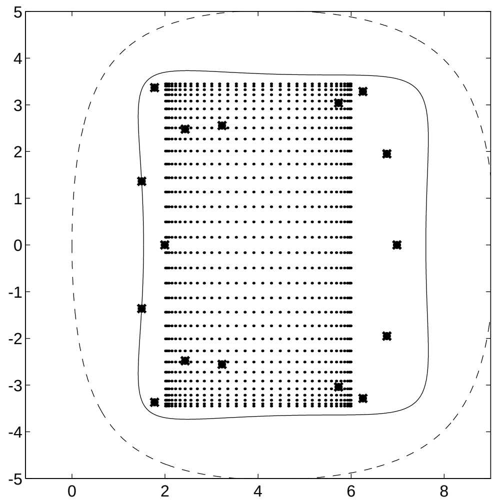

FIG. 5.2. *4-step level lines for Example 5.2, random right hand side*

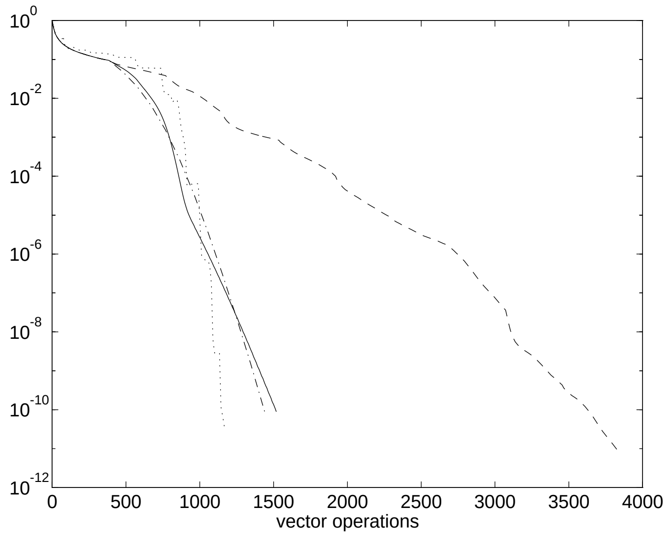

FIG. 5.3. *convergence behavior for Example 5.2, random right hand side*

vectors are chosen to be the same in our implementation. These are all iterative methods which involve matrix-vector multiplications only with A, and not with A^T, and require different amounts of saxpy operations and inner products per step. In Figure 5.3, the convergence of these iterative methods is shown in terms of vector operations, i.e., the equivalent in floating point operations of one saxpy. On vector and parallel computers, however, inner products may require much more time than is reflected by just one vector operation. In Table 5.6, we therefore list separately the number of matrix-vector multiplications, saxpys, and inner products required to reduce the initial residual by a factor of 10^{-10}.

An interesting phenomenon occurs when we start the Arnoldi process with $f = 1$ (cf. (5.2)) and

TABLE 5.6
operation counts for Example 5.2, random right hand side

	matrix-vector	saxpys	inner products
adaptive k-step	142	656	152
hybrid GMRES	192	328	152
restarted GMRES	160	1520	1520
TFQMR	106	424	212

with a zero initial guess. At first, the information obtained from 16 Arnoldi steps is not very reliable, as can be seen in Figure 5.4. The algorithm initially chooses the 1-step (first-order Richardson) method since this one has the smallest cost factor of all available k-step methods at this point (cf. Table 5.7). Based on the new information obtained in the course of this iteration, the parameters and also the degree k of the method are then adaptively changed. As shown in Figure 5.5, this finally leads to a k-step iteration which converges reasonably well.

TABLE 5.7
k-step convergence and cost factors for Example 5.2 with respect to 16 Ritz values, $f = 1$, zero initial guess

k	κ	cost factor
1	0.9592	336
2	0.9587	385
3	0.9595	448
4	0.9600	513
5	0.9610	580
6	0.9589	605
7	0.9591	672
8	0.9609	754

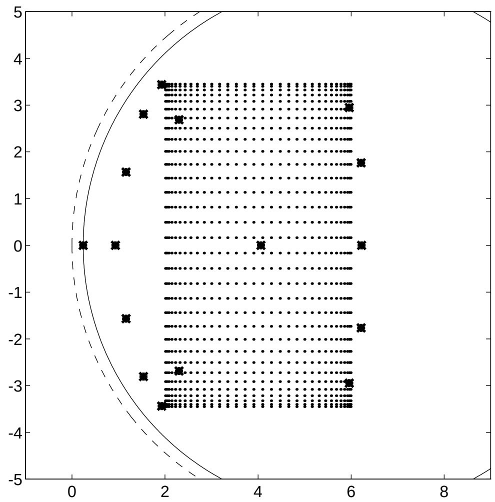

FIG. 5.4. *1-step level lines for Example 5.2, $f = 1$, zero initial guess*

It can be observed in the convergence graph of Figure 5.5 that the adaptive k-step method outperforms GMRES(16) in terms of vector operations, for this example. We wish to stress once more, at this point, that the comparison is even more favorable for the k-step method if inner products are more expensive than saxpys, as is frequently observed on vector and parallel computers. This

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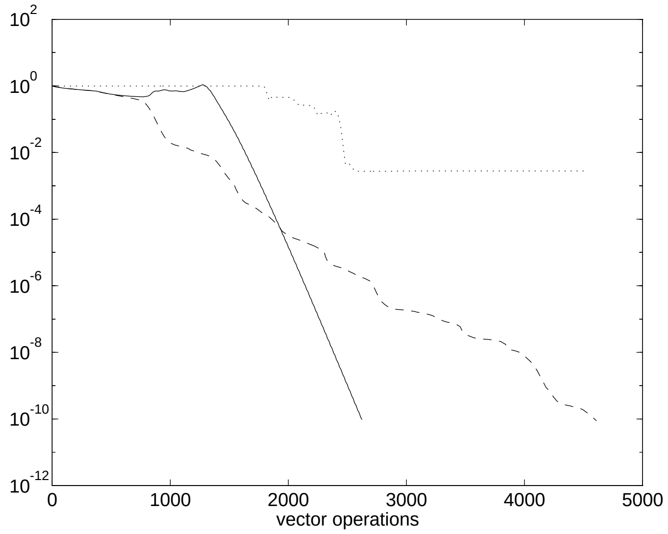

FIG. 5.5. *convergence behavior for Example 5.2, $f = 1$, zero initial guess*

is again reflected in Table 5.8, where the numbers of matrix-vector multiplications, saxpys, and inner products, are listed separately. Transpose-free QMR, again with both starting vectors being the same, did not show any sign of convergence after 1000 iterations for this example. Applying the minimal residual polynomial (of degree 16) implicitly constructed by GMRES in the form of a Richardson iteration, also did not lead to a convergent iteration here.

TABLE 5.8
operation counts for Example 5.2, $f = 1$, zero initial guess

	matrix-vector	saxpys	inner products
adaptive k-step	248	959	456
restarted GMRES	192	1824	1824

6. Conclusions. We have studied and tested here adaptive implementations of k-step methods for the iterative solution of nonsymmetric systems of real linear equations. These methods are generalizations of the well-known Chebyshev (2-step) iterative method. They are based on parameters which have to be computed by solving certain minimization problems with respect to points (representing the shape of the spectrum) in the complex plane. We have proposed an algorithm to compute near-best k-step parameters. Furthermore, we show that k-step methods can easily be implemented in an adaptive fashion in order to update the information on the matrix during the course of the iteration. The most important contribution of this paper is to illustrate that k-step methods for $k > 2$ converge in situations where the Chebyshev method does not. This is shown in Example 5.1 where the spectrum of the underlying matrix is not contained in the open right half-plane. Our limited numerical experiments also suggest that k-step methods may be competitive with other Krylov subspace methods, such as restarted GMRES, or the hybrid GMRES algorithm by Nachtigal, Reichel and Trefethen, in terms of operations required to reduce the initial residual by a certain factor. These comparisons, however, should be regarded as preliminary and more extensive testing on more realistic problems (including preconditioning) has to be done. Since the k-step iteration is inner-product-free (i.e., the computation of inner products is required only during those phases of the algorithm that collect new information), it is also attractive for use on vector and parallel computers.

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