SANDIA REPORT

SAND89-8691
Unlimited Release
Printed November 1989

Operator Coefficient Methods for Linear Equations

Invited for publication by SIAM Journal on Matrix Analysis Applications

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Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94551
for the United States Department of Energy
under Contract DE-ACO4-76DP00789

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Operator Coefficient Methods for Linear Equations*

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Abstract

New iterative methods for solving linear equations are presented that are easy to use, generalize good existing methods, and appear to be faster. The new algorithms mix two kinds of linear recurrence formulas. Older methods have either high order recurrence formulas with scalars for coefficients, as in truncated orthomin, or have 1st order recurrence formulas with matrix polynomials for coefficients, as in restarted gcr/gmres. The new methods include both: high order recurrence formulas and matrix polynomials for coefficients. These methods provide a trade-off between recurrence order and polynomial degree that can be exploited to achieve greater efficiency. Convergence results are obtained for both constant coefficient and varying coefficient methods.

* Invited for publication by SIAM Journal on Matrix Analysis and Applications.

Acknowledgements

I thank the program and organizing committees of the SIAM Conference on Sparse Matrices at Salishan Lodge in May 1989 for choosing an iconoclastic abstract for the keynote address.

I thank Dr. S. F. Ashby for many conversations which clarified the current literature, Prof. A. T. Chronopoulos and Prof. L. N. Trefethen for discussing their work, and Prof. H. C. Elman and Prof. P. E. Saylor for help with bibliographic matters.

Thanks also to Dr. S. F. Ashby, Dr. L. A. Bertram, Dr. J. M. Harris, Dr. J. F. Lathrop, Mr. S. L. Lee, Dr. J. C. Meza, Dr. L. R. Petzold and Prof. P. E. Saylor for reading the manuscript. Their patience much improved this paper.

Contents

1. Introduction

This paper develops a new class of iterative methods for solving linear equations. The new algorithms are easy to use, they generalize good existing methods, and they appear to be faster.

The new class of algorithms combines the essential features of several methods, in the following way. When many known algorithms are defined very simply, their sequences of approximate solutions can be seen to satisfy recurrence formulas of two types. Either the recurrence formulas have high orders and scalar coefficients, as in truncated orthomin, or the recurrence formulas have order 1 and polynomials of matrices for coefficients, as in restarted gcr/gmres. The new methods are the generalization to formulas that mix the two types of recurrences.

Methods in the new class build solutions from linear combinations of vectors using operators for coefficients, that is, using polynomials of matrices. The solution sequences therefore are vector linear recurrences whose coefficients are linear transformations, whence the name *operator coefficient methods*. The choice of coefficients leads to many, mostly unexplored variations.

A convenient, and in older methods, a frequent choice of coefficients repetitively solves a simple minimization problem. A new convergence result proves this choice of coefficients often results in convergence and establishes upper bounds on the convergence rates. An examination of the parameters that govern the convergence rates and some numerical experiments suggest that the new methods are faster than those currently in use. Moreover, it is suggested that both old and new algorithms may be better implemented by means of well-established, least-squares procedures.

These are the paper's major results. First, a simple characterization of iterative methods is proposed that unifies many algorithms. Similar descriptions are known for some algorithms, but they have not been systematically applied to others. Second, a spectrum of new iterative methods is found to lie between those of high recurrence order such as truncated orthomin, and those of high polynomial degree such as restarted gcr/gmres. Third, many of the algorithms are observed to have identical convergence rates. For the same convergence rate, there results a trade-off between degree and order that can be exploited to optimize efficiency. Fourth, new convergence results are proved for both constant coefficient and varying coefficient methods.

The paper's organization follows the steps which led to discovery of the new methods. First, iterative algorithms are surveyed from the historical point of view. Even those familiar with the subject may find this survey interesting. Then, some algorithms are restated in a very simple form. It is suggested this form has pedagogical and practical advantages. Two new generalizations come from it. One is a further simplification to a new class of inhomogeneous methods. Their convergence cannot be explained by existing analytical tools, nor is it analyzed here. The second and more important generalization is to operator coefficient methods. These have both homogeneous and inhomogeneous forms. A straightforward implementation for one choice of operator coefficients is proposed, and sufficient conditions for convergence are found. Finally, necessary and sufficient conditions for convergence of constant coefficient methods are found. To improve readability, appendices contain the proofs of theorems and descriptions of numerical experiments.

Chronopoulos and Gear [5] [6] [8] have been led by other considerations to derive some algorithms in the new class of methods, and their work-in-progress examines more [7]. Their work should be consulted for additional insights.

2. Survey

This section surveys the iterative methods to be analyzed in the sequel. The survey is mostly historical and phenomenological, with several omissions and some rearrangement. Those who expect to read the paper in one sitting or who are familiar with the subject may prefer to begin at Section 3 and to consult this section as needed.

Iterative methods are prescriptions for building sequences $x_0\ x_1\ x_2\ \ldots\ x_n\ \ldots$ that converge to the solution of $Ax = y$. If the prescriptions differ but the sequences are the same then the methods are the same, so some prescriptions might be better than others for the same method. The word *prescription* is new in this context.

What appears to be the natural progression of ideas for iterative algorithms involves the manner of choosing various coefficients and parameters to build the sequences. The oldest iterative methods are *incomplete* because their parameters must be selected from ancillary information. Algorithms in the second phase of development make automatic choices that are *globally correct* in some sense for some matrices. Methods in the third phase choose coefficients that are *suboptimal* but serviceable for more matrices.

The survey is bounded as follows. The first limitation is to *polynomial* methods. Each term of the sequence equals a linear combination of other vectors with coefficients that are polynomials of A. The second limitation is to polynomials *only* of A. If preconditioners are used, then A must be the result of any preconditioning matrix multiplications. The third limitation is to amounts of space and time per algorithm step limited *independent* of the step number. This means not all the preceding solutions, residuals, or whatever are available to build the next approximate solution.

The following notational conventions are used throughout. The *exact solution* of $Ax = y$ is x_*. The *error* in x_n is $e_n = x_* - x_n$. The *residual* of x_n is $r_n = y - Ax_n$. Note that $Ae_n = r_n$. Symbols with negative subscripts equal zero, and matrix-vector norms are the 2-norm, unless stated otherwise. Complex numbers are assumed. The *Hermitian part* of A is $(A^* + A)/2$. The *set of eigenvalues* of the matrix H is $\lambda(H)$.

2a. Incompletely Specified Methods

Richardson's 1st Order Method, 1910. *Iterate from* x_0.

$$x_{n+1} = \alpha_n r_n + x_n$$

Richardson's paper [43] makes interesting reading from the turn of the century. *Residual polynomials*

$$P_n(X) = \prod_{j=1}^{n} (1 - \alpha_j X)$$

have been used to understand this and other methods because they provide formulas for the residuals and the errors.

$$r_n = P_n(A)r_0 \qquad e_n = P_n(A)e_0$$

The many papers such as [41] on the proper choice of coefficients are outside the scope of this survey. If all the coefficients $\alpha_0, \alpha_1, \alpha_2, \ldots$ equal the same α, then the

method converges for all y and x_0 exactly when all the eigenvalues of A lie strictly inside the circle through 0 around $1/\alpha$ in the complex plane.

The history of iterative methods swings like a pendulum between two extremes of fashion. On the one side are the basic iterations surveyed here, on the other side are things now called preconditioners. *Preconditioning* replaces $Ax = y$ by $BAx = By$ where B is an approximate inverse for A. The pendulum started with Richardson's 1st order method, and the first reversal probably occurred when interest reverted to relaxation schemes, some of which are much older if their appellations can be believed.

The classic preconditioners were developed for use with the simplest 1st order method, for $\alpha_n = 1$ and $x_{n+1} = r_n + x_n$. They *split* the matrix $A = L + D + U$ into its diagonal and triangular parts, and choose B as follows.

D^{-1}	Jacobi, 1845
$(D+L)^{-1}$	Gauss-Seidel, 1873
$(\frac{1}{\omega}D+L)^{-1}$	SOR, Successive Overrelaxation, 1950
$\frac{2-\omega}{\omega}(\frac{1}{\omega}D+U)^{-1}D(\frac{1}{\omega}D+L)^{-1}$	SSOR, Symmetric SOR, 1950

G. E. Forsythe said Gauss-Seidel was not known to Gauss and not recommended by Seidel [30], so the very old references in this and [48] [53] [62] must be consulted to see how preconditioners predating Richardson's method, or at least Richardson's description of his method, were conceived. These and other *relaxation methods* are now viewed as a class of preconditioners. SOR was invented independently by Frankel [21] and Young [59] [60], and SSOR by Aitken [1]. In the 1950's and 60's many matrices and preconditioners were found that make Richardson's method converge. They are described by Golub [22], Golub and Varga [23] [24], Varga [53], Young [61] and many others.

2nd Order Method, (1950) 1958. *Iterate from* x_0

$$x_{n+1} = \alpha_n r_n + \beta_n x_n + \gamma_n x_{n-1}$$

in which $\beta_0 = 1$ *and* $\beta_n + \gamma_n = 1$.

Frankel [21] invented this method in 1950 and named it after Richardson. He was deferential to a fault because in the same paper he invented SOR and named it after Liebmann. Frankel and many others omit the name of the third coefficient. Stiefel [50] makes $\gamma_n = 1 - \beta_n$ appear to be a natural consequence of normalization. The conditions $\beta_0 = 1$ and $\beta_n + \gamma_n = 1$ enable the following analysis. With them the familiar residual polynomials exist

$$r_n = P_n(A)r_0 \qquad e_n = P_n(A)e_0$$

and can be built from

$$P_0(X) = 1 \qquad P_{n+1}(X) = -\alpha_n X P_n(X) + \beta_n P_n(X) + \gamma_n P_{n-1}(X)$$

just like normalized orthogonal polynomials. Stiefel may have been the first to describe the method's possibilities when he suggested consulting the theory of orthogonal polynomials to find appropriate coefficients.

Chebyshev Iteration, (1957) 1975. *Iterate from* x_0

$$x_{n+1} = \alpha_n r_n + \beta_n x_n + (1 - \beta_n) x_{n-1}$$

in which

$$\alpha_0 = 1/d \qquad \beta_0 = 1$$

$$\alpha_n = \frac{2\,T_n(d/c)}{c\,T_{n+1}(d/c)} \qquad \beta_n = \frac{2d\,T_n(d/c)}{c\,T_{n+1}(d/c)}$$

where T_n *is the* n^{th} *Chebyshev polynomial of the first kind.*

The Chebyshev iteration is the 2nd order method with residual polynomials

$$P_n(X) = \frac{T_n\left(\frac{d-X}{c}\right)}{T_n\left(\frac{d}{c}\right)}.$$

Varga [52] derived the method differently by building rapidly converging sequences from more slowly converging ones. Manteuffel [35] [36] [37] extended the method beyond symmetric positive definite matrices and coined the present name. The iteration converges for all y and x_0 exactly when all the eigenvalues of A lie strictly inside the ellipse through 0 with foci $d \pm c$ in the complex plane.

Stationary 2nd Order Method, 1982. *Iterate from* x_0 *and* x_{-1}.

$$x_{n+1} = \alpha r_n + \beta x_n + (1 - \beta) x_{n-1}$$

Iterative methods and linear recurrences are *stationary* when the coefficients are independent of n. The handful of papers on the stationary 2nd order method seek coefficients that optimize convergence for a given matrix. The answer to the simpler inverse question—which matrices converge for a given pair of coefficients?—can be obtained from [38] and a few napkins. Convergence occurs for all y and x_0 exactly when all the eigenvalues of A lie strictly inside the ellipse through 0 with foci

$$\frac{\beta}{\alpha} \pm \frac{2\sqrt{\beta - 1}}{\alpha}.$$

Moreover, the Chebyshev iteration's coefficients for these foci converge to the stationary coefficients.

2b. Completely Specified, Terminating Methods

By the time 2nd order methods were completely understood, the pendulum had already swung toward iterations with completely specified coefficients. The next method is the namesake for the entire class.

Conjugate Gradient Algorithm, (1952) 1971. *Iterate from* x_0.

$$p_n = r_n - \frac{{p_{n-1}}^* A r_n}{{p_{n-1}}^* A p_{n-1}} p_{n-1}$$

$$x_{n+1} = x_n + \frac{{p_n}^* r_n}{{p_n}^* A p_n} p_n$$

Hestenes and Stiefel [28] drew this method from optimization theory. If A is Hermitian and positive definite, then the method searches from x_n along the *direction vector* p_n for the x_{n+1} that minimizes

$$\|e_{n+1}\|_A = \sqrt{{e_{n+1}}^* A e_{n+1}} \,.$$

It happens that the p's are A-orthogonal, the r's are orthogonal, and x_{n+1} is the global minimizer within

$$\begin{aligned} x_0 + \text{span}\,\{p_0\ p_1\ p_2\ \ldots\ p_n\} = \\ x_0 + \text{span}\,\{r_0\ r_1\ r_2\ \ldots\ r_n\} = \\ x_0 + \text{span}\,\{r_0\ Ar_0\ A^2 r_0\ \ldots\ A^n r_0\}\,. \end{aligned}$$

When the subspaces stop growing the last iterate is the exact solution. Hestenes [29] derives many algebraic identities including the few needed to establish global optimality and alternate expressions for the coefficients. Golub and O'Leary [25] provide an excellent annotated bibliography for the huge corpus.

Elaborate formulas were a disadvantage on early computers so for many years the conjugate gradient algorithm was seen as a freakish alternative to Gaussian elimination [30]. By 1971 technological improvements enabled Reid [42] to view the algorithm as an iterative method and to obtain acceptable solutions after comparatively few steps. A curious tribute to Reid is that his paper is no longer read because his ideas are so completely accepted.

The matrices for which the conjugate gradient iteration finds an exact solution for all y and x_0 are the *terminating class*. This terminology is new. Preconditioning by A^* yields $A^*Ax = A^*y$ with A^*A in the terminating class but with squared condition number. Faber and Manteuffel [17] [18] [19] answered a challenge of G. H. Golub and found the terminating classes for many polynomial methods based on A alone. The Russian literature contains a related announcement at about the same time [55]. Unfortunately, all the classes are severely restricted. If the Hermitian part of A is positive definite, then Joubert and Young [32] show from the work of Faber and Manteuffel that the conjugate gradient algorithm terminates for all y and x_0 exactly when either $A^* = P(A)$ where $P(X)$ is a polynomial of degree at most 1, or $P(A) = 0$ where $P(X)$ is a nonzero polynomial of degree at most 2. The direction vectors' A-orthogonality must be reinterpreted in the non-Hermitian case.

Conjugate Residual Algorithm, (1955) 1970. *Iterate from* x_0.

$$p_n = r_n - \frac{{p_{n-1}}^* A^* A r_n}{{p_{n-1}}^* A^* A p_{n-1}} p_{n-1}$$

$$x_{n+1} = x_n + \frac{{p_n}^* A^* r_n}{{p_n}^* A^* A p_n} p_n$$

This algorithm has an interesting genealogy. Hestenes and Stiefel allude to it [28], but Stiefel describes it fully without naming it [49], and Luenberger finally names it when he reinvents it [33]. The algorithm is one of many variations of the conjugate gradient algorithm with similar properties. This one uses a different inner product. If A is Hermitian and positive definite, then the p's are A^*A-orthogonal, the r's are A-orthogonal, and x_{n+1} is the global minimizer of $\|r_{n+1}\|$ within

$$\begin{aligned} x_0 + \text{span}\,\{p_0 \;\; p_1 \;\; p_2 \;\; \ldots \;\; p_n\} = \\ x_0 + \text{span}\,\{r_0 \;\; r_1 \;\; r_2 \;\; \ldots \;\; r_n\} = \\ x_0 + \text{span}\,\{r_0 \;\; Ar_0 \;\; A^2 r_0 \;\; \ldots \;\; A^n r_0\}\,. \end{aligned}$$

Remember the convention that unspecified norms are the 2-norm. Joubert and Young [32] show from the work of Faber and Manteuffel [17] [18] [19] that among matrices whose Hermitian part is positive definite, the conjugate residual algorithm has the same terminating class as the conjugate gradient algorithm.

Alternate Conjugate Residual Algorithm, 1951. *Iterate from* x_0

$$p_n = Ap_{n-1} - \frac{{p_{n-1}}^* A^* A^2 p_{n-1}}{{p_{n-1}}^* A^* A p_{n-1}} p_{n-1} - \frac{{p_{n-2}}^* A^* A^2 p_{n-1}}{{p_{n-2}}^* A^* A p_{n-2}} p_{n-2}$$

$$x_{n+1} = x_n + \frac{{p_n}^* A^* r_n}{{p_n}^* A^* A p_n} p_n$$

but choose p_0 *as in the original conjugate residual algorithm.*

This method has been invented by many, but Forsythe, Hestenes and Rosser [20] appear to be the first [11] [25]. It is the conjugate residual method with a different prescription whose terminating class is larger. Faber and Manteuffel [18] [19] show the method converges for all y and x_0 exactly when either $A^* = P(A)$ where $P(X)$ is a polynomial of degree at most 1, or $P(A) = 0$ where $P(X)$ is a nonzero polynomial of degree at most 3. These are weaker conditions than for the conjugate residual algorithm because 3 replaces 2, and more importantly, the Hermitian part of A need not be positive definite. And yet the p's are A^*A-orthogonal, and x_{n+1} is the global minimizer of $\|r_{n+1}\|$ within

$$\begin{aligned} x_0 + \text{span}\,\{p_0 \;\; p_1 \;\; p_2 \;\; \ldots \;\; p_n\} \\ = x_0 + \text{span}\,\{r_0 \;\; Ar_0 \;\; A^2 r_0 \;\; \ldots \;\; A^n r_0\} \end{aligned}$$

just like the conjugate residual algorithm.

The relative merits of the two prescriptions are not clear. The original fails for an indefinite matrix when a direction vector makes no contribution to the solution.

In this unlikely event the residuals do not change and the subsequent direction vectors lie within the span of the previous. The alternate version succeeds because it builds the direction vectors from a self-contained recurrence. In some sense the alternate prescription is an analytic continuation of the original. But the theoretically more powerful prescription amounts to evaluating the Lanczos recurrence, which may be more sensitive to rounding errors.

The effects of rounding errors are a major disappointment for all these algorithms. Loss of orthogonality and failure to terminate are the most easily observed symptoms. The conjugate gradient algorithm should have $p_i{}^* A p_j = 0$ for $i \neq j$, but in practice $p_i{}^* A p_j / (\|p_i\|_A \|p_j\|_A)$ grows exponentially with $|i-j|$. Figure 1 makes the more difficult comparison between the numerically computed direction vectors and those that would be obtained from error-free arithmetic. This data may be the first of its kind in print. The formulas for the direction vectors evidently are unstable because they magnify the small perturbations due to rounding error. Figure 2 shows the resulting delayed convergence. Greenbaum has a detailed analysis of the retarded convergence [27], but no universal, inexpensive cure is known.

Interest in the conjugate gradient algorithm was intense for a time. Many terminating algorithms were proposed with enlarged terminating classes. *Generalized* refers indiscriminately to these methods for which there is no consistent naming convention. The generalized conjugate gradient algorithm [9] [10] [58] established the use of very different inner products and to some extent prompted the work of Faber and Manteuffel. Ashby, Manteuffel and Saylor classify many generalizations of this kind [3].

Some terminating generalizations of the conjugate gradient algorithm have mostly theoretically use. The analyses of Faber and Manteuffel and of Joubert and Young actually proceed by seeking conditions under which the original algorithm is equivalent to a generalized one that uses all the direction vectors to build the next. The same generalization can be made of the conjugate residual algorithm.

Generalized Conjugate Residual Algorithm, 1982. *Iterate from* x_0.

$$p_n = r_n - \sum_{i=1}^{n} \frac{p_{n-i}{}^* A^* A r_n}{p_{n-i}{}^* A^* A p_{n-i}} p_{n-i}$$

$$x_{n+1} = x_n + \frac{p_n{}^* A^* r_n}{p_n{}^* A^* A p_n} p_n$$

Formulas of this kind may be traced to Arnoldi [2], but this algorithm is from Elman [14] and Eisenstat, Elman and Schultz [13]. Its terminating class includes all matrices with positive definite Hermitian parts. The method itself is impractical, and is outside the bounds of the present survey, because all the previous direction vectors must be saved. It can be made practical either by *truncating* the sum, or by *restarting* the iteration, as follows.

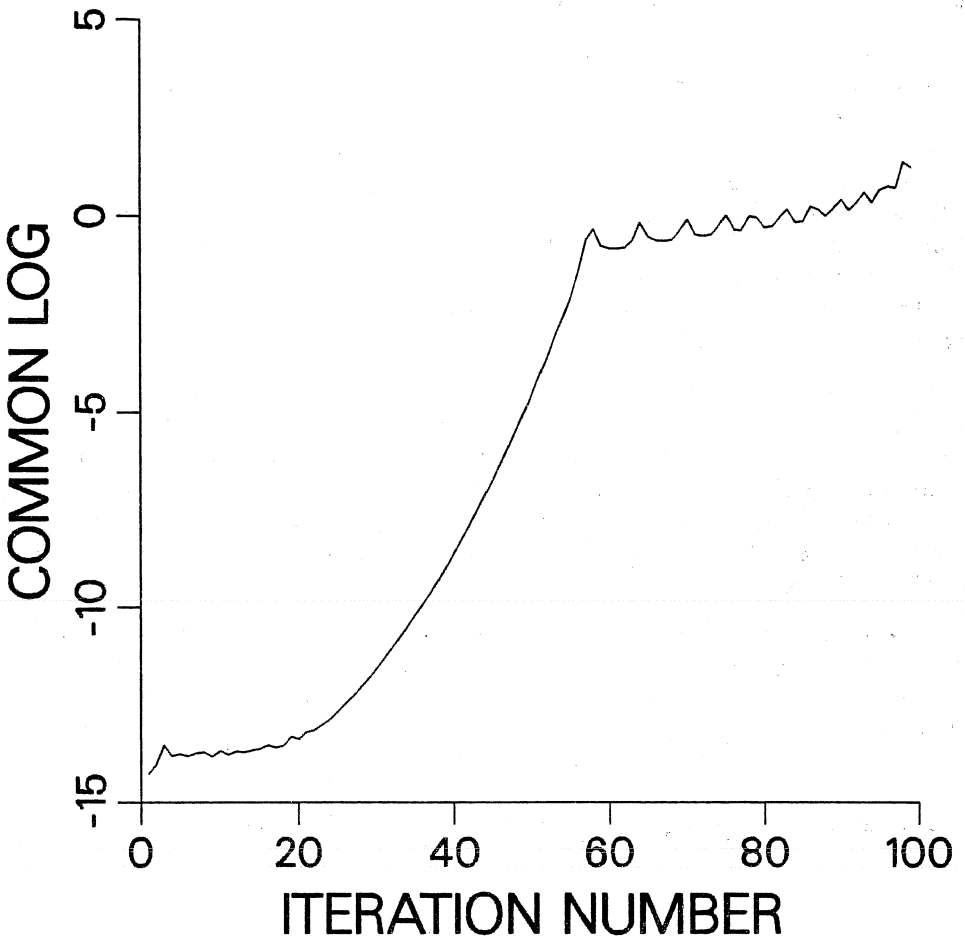

Figure 1. *2-norm relative errors in the computed basis vectors of the conjugate gradient algorithm for a system of order* 100. *Appendix 2 and Section 2b explain the calculations.*

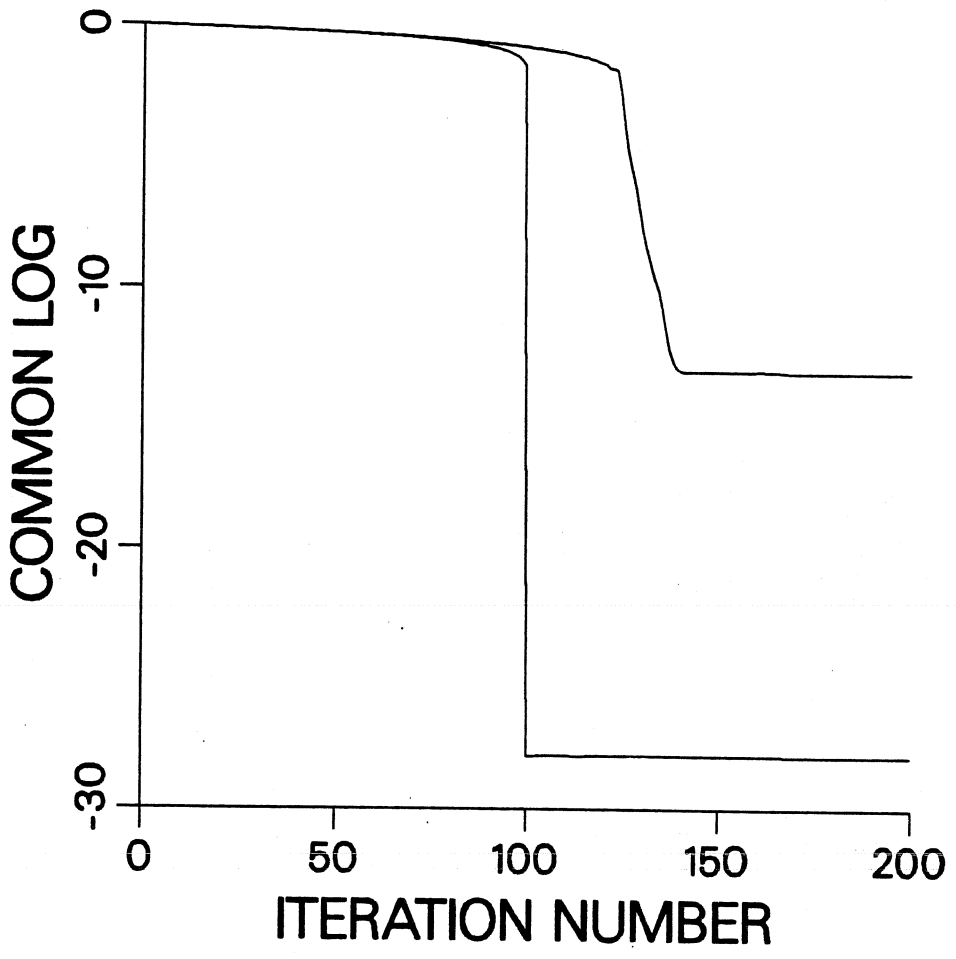

Figure 2. *Relative A-norm solution errors for the system of Figure 1. The upper curve is for single precision and the lower for reorthogonalized double precision. Appendix 2 and Section 2b explain the calculations.*

2c. Completely Specified, Non-Terminating Methods

Orthomin(m), 1976. *Iterate from* x_0.

$$p_n = r_n - \sum_{i=1}^{m} \frac{{p_{n-i}}^* A^* A r_n}{{p_{n-i}}^* A^* A p_{n-i}} p_{n-i}$$

$$x_{n+1} = x_n + \frac{{p_n}^* A^* r_n}{{p_n}^* A^* A p_n} p_n$$

Vinsome [54] invented this *truncated* algorithm and made non-terminating or suboptimal convergence respectable again. Elman [14] and Eisenstat, Elman and Schultz [13] prove convergence for all y and x_0 whenever the Hermitian part of A is positive definite. Specifically, they prove

$$\|r_{n+1}\| \leq \|r_n\| \sqrt{1 - \left[\frac{\min|\lambda(A^* + A)|}{2\|A\|}\right]^2} < \|r_n\|.$$

They also show each set of $m+1$ consecutive direction vectors is A^*A-orthogonal, and x_{n+1} minimizes $\|r_{n+1}\|$ within

$$x_{n-m\wedge 0} + \text{span}\,\{p_{n-m} \;\cdots\; p_{n-2}\; p_{n-1}\; p_n\}.$$

The notation is rigorously correct because things with negative subscripts vanish and the wedge in $x_{n-m\wedge 0}$ means the maximum of $n-m$ and 0. It is an open question why the suboptimal convergence results ignore m and exclude the Hermitian indefinite case for which the alternate conjugate residual algorithm has terminating convergence.

The truncated algorithm is expected to have dependable convergence for many matrices rather than terminating convergence for a few. As m increases the terminating class grows beyond that of the conjugate residual method, but only through the addition of matrices having at most m^2 distinct eigenvalues [18] [19] [32]. Termination also occurs, of course, for m so impractically large that the method reverts to the generalized conjugate residual method.

As with the conjugate residual algorithm, there is an alternate version that generates the direction vectors independently of the residuals. Saad and Schultz survey many equivalent prescriptions [46]. Saad develops some of these algorithms himself, and names the class *incomplete orthogonalization methods* [44]. Jea and Young [31] also develop a broad class of methods and also provide extensive references to other work. In their terminology, the original conjugate residual algorithm is an *orthomin* and the alternate is an *orthodir*, both with $m = 1$ and with specific choices for inner products and the like. Faber and Manteuffel [17] [18] [19] actually treat the alternate prescriptions, but Joubert and Young [32] and Ashby, Manteuffel and Saylor [3] carefully observe the distinction.

Gcr(k), Restarted Generalized Conjugate Residual Method, 1979. *Iterate from* x_0, *and for each* x_n *obtain* x_{n+1} *by building the sequence*

$$x_n = x_{(0)} \quad x_{(1)} \quad x_{(2)} \quad \cdots \quad x_{(k+1)} = x_{n+1}$$

by iterating the generalized conjugate residual algorithm from $x_{(0)}$ *to* $x_{(k+1)}$

$$p_{(j)} = r_{(j)} - \sum_{i=1}^{j} \frac{p_{(i-1)}{}^* A^* A r_{(j)}}{p_{(i-1)}{}^* A^* A p_{(i-1)}} p_{(i-1)}$$

$$x_{(j+1)} = x_{(j)} + \frac{p_{(j)}{}^* A^* r_{(j)}}{p_{(j)}{}^* A^* A p_{(j)}} p_{(j)}$$

in which the subscripts in parentheses indicate dependence on n.

The idea of *restarting* an algorithm contrasts with truncating in orthomin(m). It is the theory that jiggling the ignition recharges the battery and may be due to several people. Luenberger [34] restarts the conjugate gradient algorithm to circumvent numerical difficulties, while Eisenstat, Elman, Schultz and Sherman [12] [13] [14] restart the generalized conjugate residual method to conserve memory space. They show that gcr(k) minimizes $\|r_{n+1}\|$ within

$$x_n + \text{span}\left\{r_n \;\; Ar_n \;\; A^2 r_n \;\; \ldots \;\; A^k r_n\right\}$$

and converges when the Hermitian part of A is positive definite.

Like truncated orthomin, restarted gcr is expected to have dependable convergence for many matrices rather than terminating convergence for a few. And again there is an alternate prescription. This one additionally makes the direction vectors orthogonal with respect to the Euclidean inner product rather than the A^*A inner product.

Gmres(k), Restarted Generalized Minimum Residual Algorithm, 1983. *Iterate from* x_0, *and for each* x_n *build the orthonormal sequence*

$$\frac{r_n}{\|r_n\|} = p_{(1)} \quad p_{(2)} \quad p_{(3)} \quad \cdots \quad p_{(k+1)}$$

from Arnoldi's recurrence equations

$$h_{(j+1,j)}\, p_{(j+1)} = A\, p_{(j)} - \sum_{i=1}^{j} h_{(i,j)}\, p_{(i)}$$

with appropriately chosen $h_{(i,j)}$*'s, and then chose* $\alpha_{(j)}$*'s to minimize*

$$\left\| \, \|r_n\| \, e_1 - [h_{(i,j)}]\,[\alpha_{(j)}] \, \right\|$$

in which e_1 *is the first column of an identity matrix and* $[h_{(i,j)}]$ *is the* $(k+1) \times k$ *matrix of recurrence coefficients, and finally construct*

$$x_{n+1} = x_n + \sum_{j=1}^{k} \alpha_{(j)}\, p_{(j)}.$$

The subscripts in parentheses indicate dependence on n.

Saad and Schultz [45] [47] developed this most widely used version of restarted gcr. It uses an alternate prescription to generate the normalized direction vectors,

with the precise choice of $h_{(i,j)}$'s clear and mercifully omitted. The coefficients for x_n are selected from the small matrix that describes the action of A on the orthonormal basis. Nevertheless, gmres(k) minimizes $||r_{n+1}||$ within

$$x_n + \text{span}\ \{r_n\ \ Ar_n\ \ A^2r_n\ \ \ldots\ \ A^{k-1}r_n\}$$

just like gcr($k-1$). Both prescriptions sometimes have difficulty solving the least squares problem, and other prescriptions have been proposed [56] [57].

Note the multiple names. Gcr($k-1$) is gmres(k). The first generalizes the conjugate residual algorithm and the second generalizes the minimum residual algorithm. So there is yet another line of development which leads to the same methods. But this is too broad a subject for discussion.

3. Simplification

The completely specified algorithms in the survey can be reduced to simpler but equivalent form. Here, all inessential notation is removed to leave what may be the vital core. This naive approach leads to useful generalizations in subsequent sections, and even to useful implementations. The simplified algorithms are strikingly similar. Each chooses its next solution from a small *selection space*, and uses a minimization problem as the *selection criterion*.

Another form of the conjugate gradient algorithm discards the direction vectors and reveals it to be a 2nd order method.

$$x_{n+1} = \alpha_n r_n + \beta_n x_n + (1-\beta_n)x_{n-1}$$

This version has several sources. One builds the coefficients recursively, and is attributed to Engeli, Ginsberg, Rutishauser and Stiefel [16] by [63], and to Rutishauser alone by [42]. Hestenes [29] cites a form called *paratan* with a geometric interpretation and explicit coefficient formulas [48].

$$\alpha_n = \frac{||r_{n-1}||^2||r_n||^2}{||r_{n-1}||^2(r_n^*Ar_n) + ||r_n||^2(r_{n-1}^*Ar_n)}$$

$$\beta_n = \frac{||r_{n-1}||^2(r_n^*Ar_n)}{||r_{n-1}||^2(r_n^*Ar_n) + ||r_n||^2(r_{n-1}^*Ar_n)}$$

These formulas too can be discarded because theorems say they make $||e_{n+1}||_A$ globally minimal, and therefore locally minimal. In this way a simple minimization criterion concisely replaces many elaborate formulas. This interpretation succinctly characterizes both the conjugate gradient algorithm and its cousin.

Simplest Conjugate Gradient Algorithm. *Iterate from* x_0.

minimize $||e_{n+1}||_A$ *over span* $\{r_n\ \ x_n\ \ x_{n-1}\}$
so coefficients of x_n *and* x_{n-1} *sum to* 1

Simplest Conjugate Residual Algorithm. *Iterate from* x_0.

minimize $||r_{n+1}||_2$ *over span* $\{r_n\ \ x_n\ \ x_{n-1}\}$
so coefficients of x_n *and* x_{n-1} *sum to* 1

The starting point for a simpler version of orthomin(m)

$$p_n = r_n - \sum_{i=1}^{m} \frac{{p_{n-i}}^* A^* A r_n}{{p_{n-i}}^* A^* A p_{n-i}} p_{n-i}$$

$$x_{n+1} = x_n + \frac{{p_n}^* A^* r_n}{{p_n}^* A^* A p_n} p_n$$

is the work of Elman [14] and Eisenstat, Elman and Schultz [13]. They show if the Hermitian part of A is positive definite, then x_{n+1} minimizes $\|r_{n+1}\|$ within

$$x_{n-m\wedge 0} + \text{span } \{p_{n-m} \ \cdots \ p_{n-2} \ p_{n-1} \ p_n\}$$

and the coefficient in the formula for x_{n+1} can't vanish. The notation is rigorously correct because things with negative subscripts vanish and the wedge in $x_{n-m\wedge 0}$ means the maximum of $n-m$ and 0. The formula for p_n means r_n can replace p_n inside the span. The formula for x_{n+1-j} means $(x_{n+1-j} - x_{n-j})$ can replace p_{n-j}. With these substitutions the affine space becomes

$$x_{n-m\wedge 0} + \text{span} \left\{ \ (x_{n+1-m} - x_{n-m}) \ \cdots \ (x_{n-1} - x_{n-2}) \ \ (x_n - x_{n-1}) \ \ r_n \ \right\}$$

from which $(x_{n+1-j} - x_{n-j})$ vanishes if $n-j < 0$. The x-coordinates of each vector in the span sum to zero, and the affine space adds $x_{n-m\wedge 0}$, so the x-coordinates of each vector in the affine space sum to 1.

Simplest Orthomin(m). *Iterate from* x_0

$$\begin{array}{c} \textit{minimize } \|r_{n+1}\| \textit{ over span } \{r_n \ \ x_n \ \ x_{n-1} \ \ x_{n-2} \ \cdots \ x_{n-m}\} \\ \textit{so coefficients of } x_n \ \ x_{n-1} \ \ x_{n-2} \ \cdots \ x_{n-m} \textit{ sum to } 1 \end{array}$$

This definition of orthomin(m) may be new, but the simplest form of gcr(k−1)/ gmres(k) is well known and needs no derivation. Table 1 allows side-by-side comparison of the simplest versions of all these methods for the first time.

These versions are proposed as archetypes for study and use. Each prescription is a simple linear recurrence with coefficients that repetitively solve a simple minimization problem. Confusion and duplication of effort are unlikely because identity and functionality are clear at a glance. Straightforward solution of the minimization problems affords easy comparison and substitution of methods.

Table 1. *Simplest prescriptions for the survey's completely specified algorithms. Section 3 provides further explanation.*

conjugate gradient minimize $\|e_{n+1}\|_A$ over span $\{r_n \; x_n \; x_{n-1}\}$ so coefficients of x_n and x_{n-1} sum to 1.
conjugate residual minimize $\|r_{n+1}\|_2$ over span $\{r_n \; x_n \; x_{n-1}\}$ so coefficients of x_n and x_{n-1} sum to 1
orthomin(m) minimize $\|r_{n+1}\|_2$ over span $\{r_n \; x_n \; x_{n-1} \; x_{n-2} \; \ldots \; x_{n-m}\}$ so coefficients of $x_n \; x_{n-1} \; x_{n-2} \; \ldots \; x_{n-m}$ sum to 1
gcr(k−1)/gmres(k) minimize $\|r_{n+1}\|_2$ over span $\{x_n \; r_n \; Ar_n \; A^2r_n \; \ldots \; A^{k-1}r_n\}$ so coefficient of x_n equals 1

4. Inhomogeneous Methods

New methods can be derived by further simplifying the algorithms of Table 1. The resulting algorithms apparently cannot be analyzed by traditional theory, nor is a new theory offered here. These algorithms do simplify Section 5's presentation of more important generalizations.

A common feature of all the algorithms in Table 1 is the constraint that the x-coefficients sum to 1. That is, the next solution equals a linear combination of previous solutions and other things, in which the coefficients of the previous solutions sum to 1. This constraint is called the *consistency condition*, but *homogeneity condition* more accurately describes its use. With it, the formula for the next solution can be multiplied by A and subtracted from y to make an homogeneous recurrence for the residuals, and this can be multiplied by A^{-1} to make a similar recurrence for the errors. If the recurrence formulas are used to produce polynomials rather than vectors, then all the residuals and errors can be obtained formally, by multiplying the initial residual and error by these so-called residual polynomials evaluated at the matrix A.

The entire convergence theory of iterative methods rests on residual polynomials. Convergence to the solution of $Ax = y$ depends on both A and y, but the homogeneity condition allows a separation of variables in which the entries of A are more prominent than the entries of y. Convergence is equivalent to the residual polynomials having small values at the matrix eigenvalues. The incompletely specified algorithms in Section 2a need parameters that make the polynomials small independent of y. The completely specified algorithms in Sections 2b and 2c choose parameters that make the polynomials small in norms weighted by the entries of y. In both cases, convergence depends strongly on A and weakly on y.

When the algorithms are stated so simply as in Table 1, however, there is clearly no reason to impose homogeneity. It is a theoretical convenience for convergence analysis that is superfluous to the algorithms. Completely new algorithms can be derived by removing the constraint. Table 2 presents these even simpler, *inhomogeneous* algorithms. Henceforth, the original algorithms are called *homogeneous.*

Table 2. *Inhomogeneous, simplest prescriptions for the survey's completely specified methods. Section 4 provides further explanation.*

un-conjugate gradient minimize $\|e_{n+1}\|_A$ over span $\{r_n\ x_n\ x_{n-1}\}$
un-conjugate residual minimize $\|r_{n+1}\|_2$ over span $\{r_n\ x_n\ x_{n-1}\}$
un-orthomin(m) minimize $\|r_{n+1}\|_2$ over span $\{r_n\ x_n\ x_{n-1}\ x_{n-2}\ \cdots\ x_{n-m}\}$
un-gcr($k-1$)/gmres(k) minimize $\|r_{n+1}\|_2$ over span $\{x_n\ r_n\ Ar_n\ A^2r_n\ \ldots\ A^{k-1}r_n\}$

Figure 3 shows that the new, inhomogeneous methods may converge when the old, homogeneous methods do not. The selection criteria evidently find smaller minima when the selection spaces grow by removing the homogeneity constraint. This explanation is too simple, however, because it does not characterize the new convergence rate. This difficult question is not addressed here beyond the following comments. First, terminating algorithms already make globally optimal choices, so removing the constraint should not change them, at least in exact arithmetic. Second, if the recurrence coefficients of non-terminating algorithms converge to constant values, then the recurrence formulas must be homogeneous in the limit. In particular, algorithms with constant coefficients must be homogeneous.

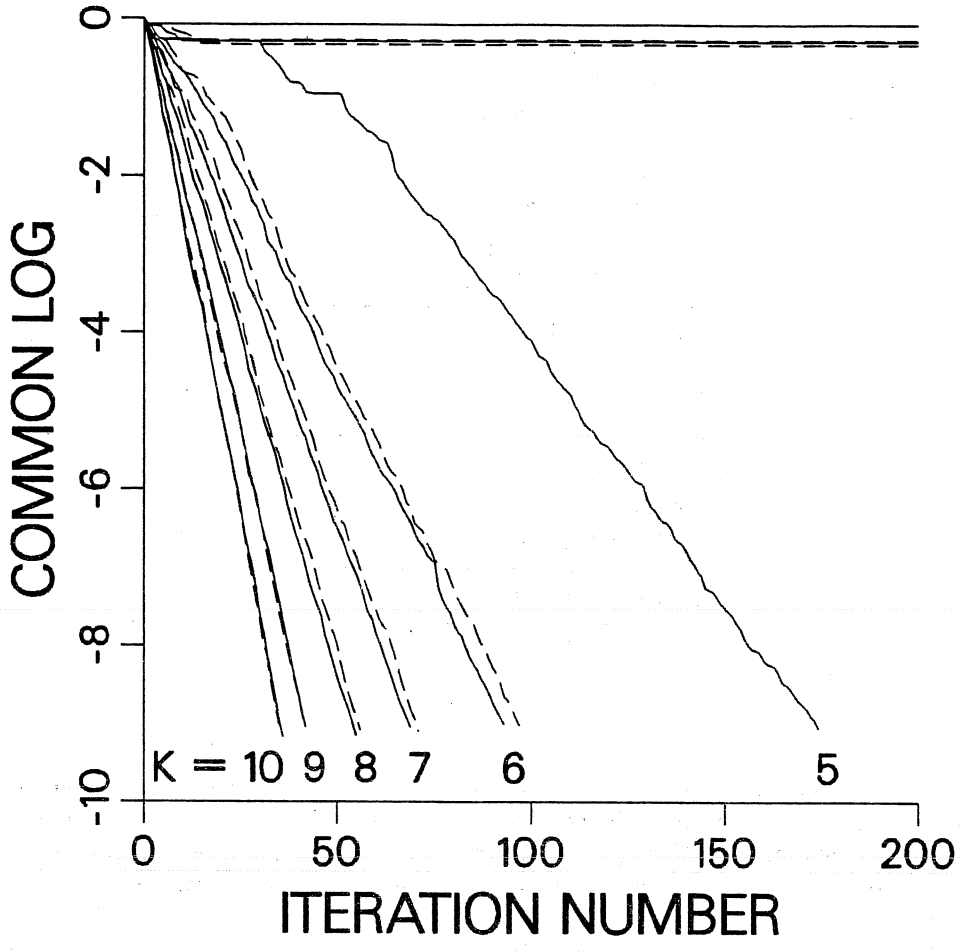

Figure 3. *2-norm relative residuals for homogeneous (dashed) and inhomogeneous (solid) gcr(k−1)/gmres(k), k = 1, 2, ..., 10, applied to one system. The two methods perform alike except for k = 5 when the original, homogeneous method stagnates and the new, inhomogeneous method converges. Appendix 2 and Section 4 explain the calculations.*

5. Operator Coefficient Methods

This paper's major observation is that new iterative methods can be derived by combining the algorithms of Table 2. The easiest way to join the algorithms is to amass their selection spaces, as follows.

The basis vectors naturally fit into a tableau. Those of the conjugate gradient algorithm and the conjugate residual algorithm occupy a corner, those of orthomin(m) add a row, and those of gcr($k-1$)/gmres(k) fill a column.

$$\begin{array}{cccccc} x_n & x_{n-1} & x_{n-2} & \cdots & x_{n-m} \\ r_n & & & & \\ Ar_n & & & & \\ \vdots & & & & \\ A^{k-1}r_n & & & & \end{array}$$

Orthomin(m) apparently gains its advantage over the conjugate residual algorithm by keeping more old solutions. It is likely the vectors of gcr($k-1$)/gmres(k) can be kept with some advantage too. The tableau does have room for many more.

$$\begin{array}{cccccc} x_n & x_{n-1} & x_{n-2} & \cdots & x_{n-m} \\ r_n & r_{n-1} & r_{n-2} & \cdots & r_{n-m} \\ Ar_n & Ar_{n-1} & Ar_{n-2} & \cdots & Ar_{n-m} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ A^{k-1}r_n & A^{k-1}r_{n-1} & A^{k-1}r_{n-2} & \cdots & A^{k-1}r_{n-m} \end{array}$$

The remainder of this paper demonstrates that better iterative methods can be created by placing some or all of these vectors into the selection spaces. The following definition of the new methods involves a change of notation because the tableau loses one column.

Oc(k, m), Operator Coefficient Methods of Degree k and Order m. *Begin from x_0 and optionally from x_{-1}, x_{-2}, ..., x_{1-m}, and choose x_n to*

$$\textit{minimize } \|r_n\|_{\textit{whatever}} \textit{ or whatever}$$

from among

$$\textit{span} \left\{ \begin{array}{cccc} x_{n-1} & x_{n-2} & \cdots & x_{n-m} \\ r_{n-1} & r_{n-2} & \cdots & r_{n-m} \\ Ar_{n-1} & Ar_{n-2} & \cdots & Ar_{n-m} \\ \vdots & \vdots & \ddots & \vdots \\ A^{k-1}r_{n-1} & A^{k-1}r_{n-2} & \cdots & A^{k-1}r_{n-m} \end{array} \right\}$$

and, in the homogeneous case, choose x_n so the x-coefficients sum to 1.

The definition above introduces a name for a generic class of old and new algorithms. Three aspects need further explanation. First, it isn't necessary to

employ all the vectors in the span. Some old algorithms do not. Second, the selection criteria is unspecified because there are so many possibilities. Some are explored in later sections. Third, since the recurrence formula has order m, it is possible to begin from m initial guesses, x_0, x_{-1}, x_{-2}, ..., x_{1-m}. In this case the operator coefficient method is not a Krylov space method.

Operator coefficient methods include many known iterative algorithms. For example, gcr($k-1$)/gmres(k) is an homogeneous oc $(k, 1)$ method minimizing the 2-norm of the residual. Orthomin(m) is an homogeneous oc $(1, m+1)$ method that also minimizes the 2-norm of the residual and has only the latest residual in the selection space. The conjugate gradient and conjugate residual algorithms are homogeneous oc $(1, 2)$ methods that minimize various norms and also have only the latest residual in the selection space. It would be interesting to find a polynomial-based iterative algorithm that is not an operator coefficient method.

Methods that employ the entire $(k + 1) \times m$ tableau may greatly reduce the matrix-vector multiplications needed to solve equations to prescribed accuracy. The convergence rate of truncated orthomin generally improves as the order, m, increases. Orthomin is a 1st degree method, $k = 1$, and similar behavior may be expected for higher degree methods, $k > 1$. Figure 4 shows convergence significantly improves by increasing m and fixing k. In this case the matrix-vector multiplications for each step are independent of m and are identical to those of gcr($k-1$)/ gmres(k). Thus, convergence quickens by solving larger minimization problems but by performing the same matrix-vector multiplications per step. Faster convergence means fewer steps, and fewer matrix-vector multiplications overall. This subject is discussed again in Section 7.

Reducing matrix-vector multiplications is a significant achievement because they can account for most of the computational work. When the matrix is randomly sparse, then matrix-vector multiplications perform random memory accesses which are comparatively slow. If the matrix is not explicitly known, as in matrix-free solution of ordinary differential equations [4], then matrix-vector multiplications require numerical differentiation of functions whose evaluation may be very slow.

Several recurrence formulas are associated with an operator coefficient method. The selection criterion

$$\text{minimize } \|r_n\|_{\text{whatever}} \text{ or whatever}$$

chooses a *coefficient tableau*

$$\begin{matrix} c_{(0,1)} & c_{(0,2)} & \cdots & c_{(0,m)} \\ c_{(1,1)} & c_{(1,2)} & \cdots & c_{(1,m)} \\ c_{(2,1)} & c_{(2,2)} & \cdots & c_{(2,m)} \\ \vdots & \vdots & \ddots & \vdots \\ c_{(k,1)} & c_{(k,2)} & \cdots & c_{(k,m)} \end{matrix}$$

which produces the next iterate

$$x_n = \sum_{j=1}^{m} c_{(0,j)} x_{n-j} + \sum_{i=1}^{k} \sum_{j=1}^{m} c_{(i,j)} A^{i-1} r_{n-j}.$$

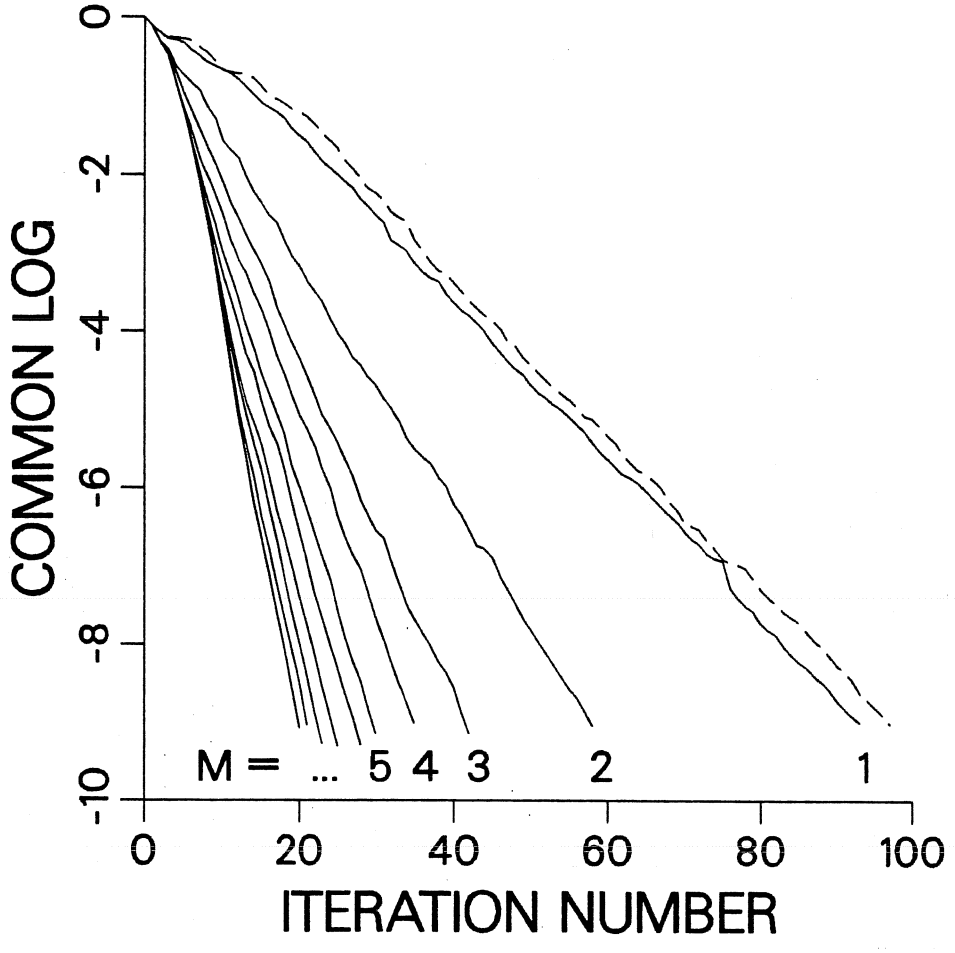

Figure 4. *2-norm relative residuals for homogeneous (dashed) gcr(5)/ gmres(6) and inhomogeneous (solid) oc(6,m), m = 1 2 ... 10, applied to the same system. Appendix 2 and Section 5 explain the calculations.*

Parenthetical subscripts in this and other formulas indicate dependence on n. The next residual can be obtained by a similar formula

$$r_n = \sum_{j=1}^{m} c_{(0,j)} r_{n-j} - \sum_{i=1}^{k} \sum_{j=1}^{m} c_{(i,j)} A^i r_{n-j} + f_n$$

$$f_n = y - \sum_{j=1}^{m} c_{(0,j)} y$$

which can be written as a recurrence formula of order m

$$r_n = P_{(1)}(A) r_{n-1} + P_{(2)}(A) r_{n-2} + \cdots + P_{(m)}(A) r_{n-m} + f_n$$

whose coefficients are operators, that is, are polynomials of degree k

$$P_{(j)}(X) = c_{(0,j)} - c_{(1,j)} X - c_{(2,j)} X^2 - \cdots - c_{(k,j)} X^k$$

evaluated at the matrix A. Whence the name, *operator coefficient method of degree k and order m*. If $c_{(0,1)} + c_{(0,2)} + \cdots + c_{(0,m)} = 1$, then the f_n's vanish and the residuals satisfy homogeneous recurrence formulas. Whence *homogeneous* and *inhomogeneous* methods. In the homogeneous case, the residuals can be expressed succinctly in terms of the initial residuals

$$r_n = P_{n,1}(A) r_0 + P_{n,2}(A) r_{-1} + P_{n,3}(A) r_{-2} + \cdots + P_{n,m}(A) r_{1-m}$$

by means of residual polynomials, $P_{n,j}(X)$, generated from the recurrence formulas

$$P_{n,j} = P_{(1)} P_{n-1,j} + P_{(2)} P_{n-2,j} + \cdots + P_{(m)} P_{n-m,j}$$

with initial values $P_{1-j,j} = 1$ and others zero. This representation for r_n is numerically correct, however, only if the recurrence formulas are stable when $X = A$.

6. Implementations

The implementation of inhomogeneous operator coefficient methods that minimize the 2-norm of the residual is considered here. This section has two parts. The first analyzes implementations of older methods, the second describes a reasonable implementation for all oc(k,m) methods. Those who are interested in the new methods may prefer to read the notation below and to begin at Section 6b.

Inhomogeneous oc(k,m) methods that minimize the 2-norm of the residual perform the following task at step n. They choose $x_n = V_n c_n$, where c_n solves the least squares problem

$$\min \|y - AV_n c_n\|_2,$$

and where V_n's columns are a basis for the selection space. The *natural basis* for the full-tableau method is the following.

$$\text{span } \{V_n\} = \text{span} \left\{ \begin{array}{cccc} x_{n-1} & x_{n-2} & \cdots & x_{n-m} \\ r_{n-1} & r_{n-2} & \cdots & r_{n-m} \\ \vdots & \vdots & \ddots & \vdots \\ A^{k-1}r_{n-1} & A^{k-1}r_{n-2} & \cdots & A^{k-1}r_{n-m} \end{array} \right\}$$

Any implementation makes three choices. The first is the basis for the selection space. This basis becomes the columns of V_n. The second choice is the basis for the least squares problem. This might be the columns of AV_n. The third choice is the process to solve the least squares problem. All the choices affect both numerical accuracy and computational efficiency. The bases might overlap to conserve storage, for example, or they might facilitate the solution process to conserve time. The chief numerical considerations are the accuracy of the bases and the accuracy of the least squares solution. A comparative analysis of all the possibilities is beyond the scope of this paper. Ashby, Manteuffel and Saylor [3], Saad and Schultz [46], Walker [56] [57] and references therein should be consulted for more implementation ideas.

6a. Some Existing Implementations

This section analyzes implementations of known methods. It reverses Section 3's simplification process, and rebuilds the algorithms with explicit justification for each implementation detail.

Like more general operator coefficient methods, gcr($k-1$) and gmres(k) solve a least squares problem, but their selection space is smaller and affine. They choose $x_n = x_{n-1} + V_n c_n$, where c_n solves

$$\min \|r_{n-1} - AV_n c_n\|_2,$$

and where

$$\text{span } \{V_n\} = \text{span} \left\{ \begin{array}{c} r_{n-1} \\ Ar_{n-1} \\ \vdots \\ A^{k-1}r_{n-1} \end{array} \right\}.$$

The gcr implementation of gcr($k-1$)/gmres(k) maintains two separate bases. It uses AV_n for the least squares basis, and it chooses V_n to be A^*A-orthogonal. Evaluation of the inner products during the orthogonalization process requires either that the columns of AV_n be saved, or that additional matrix-vector multiplications be performed. Since AV_n is Euclidean-orthogonal, the normal equations are diagonal and are easily solved. However, normal equations may solve least squares problems with accuracy less than best.

The gmres version of gcr($k-1$)/gmres(k) may be the most efficient for this method. It chooses an Euclidean-orthonormal basis for span $\{V_n\}$ that becomes an orthonormal basis for span $\{V_n\}$ + span $\{AV_n\}$ by the inclusion of one more vector. That is, $AV_n = W_n H_n$ where W_n has the columns of V_n plus one, and where the small matrix H_n is constructed along with the basis. H_n represents A under an orthonormal change of basis. If the change of basis can be computed accurately, then H_n can be used to solve the least squares problem accurately.

It is not clear whether so efficient an implementation is possible for more general operator coefficient methods. The oc $(k, 1)$ methods have the advantage of simplicity because their selection spaces involve a single group of nested Krylov spaces.

$$\text{span } \{r_{n-1}\} = K_0 \subseteq K_1 \subseteq \cdots \subseteq K_{k-1} = \text{span } \{r_{n-1} \;\; Ar_{n-1} \;\; \cdots \;\; A^{k-1}r_{n-1}\}$$

More general oc (k, m) methods have several Krylov spaces and so may not attain the efficiencies of the 1st order, $m = 1$, methods.

The usual practice with oc $(k, 1)$ methods is to recursively build orthogonal bases for the nested Krylov spaces,

$$K_{j+1} = \text{span } \{p_0 \;\; p_1 \;\; \cdots \;\; p_j \;\; p_{j+1}\} = \text{span } \{K_j \;\; p_{j+1}\},$$

in which p_{j+1} is orthogonal to K_j. Restarted gcr employs A^*A orthogonality, while restarted gmres chooses Euclidean orthogonality. Orthogonality is desired for two reasons. It is generally believed orthogonal bases provide better numerical representations for their spans, moreover, orthogonality can help solve the least squares problem.

The experience with orthomin($m-1$), an homogeneous oc $(1, m)$ method, suggests orthogonality has a third use. It may provide efficient implementations of high order, $m > 1$, methods. Like gcr/gmres, orthomin($m-1$) chooses $x_n = x_{n-1} + V_n c_n$ where c_n solves

$$\min \|r_{n-1} - AV_n c_n\|_2,$$

but in this case

$$\text{span } \{V_n\} = \text{span } \left\{ \; r_{n-1} \quad (x_{n-1} - x_{n-2}) \quad \cdots \quad (x_{n-(m-1)} - x_{n-m}) \; \right\}.$$

Orthomin($m-1$) represents this selection space by an *inventory* of A^*A-orthogonal basis vectors,

$$V_n = [\, p_{n-1} \;\; p_{n-2} \;\; \cdots \;\; p_{n-m} \,].$$

Each step maintains the basis by discarding the oldest vector and inserting the residual's component orthogonal to the others. As with gcr, A^*A-orthogonality results in diagonal normal equations for the least squares problem. The solution

update involves only the newest basis vector because previous steps account for the others. In this way, each basis vector spans exactly the difference between a pair of successive approximate solutions.

Some algorithms of Chronopoulos and Gear [5] [6] [7] [8] appear to be more general oc(k, m) methods that follow the approach taken by truncated orthomin. They build the natural basis for a Krylov space of low dimension, say k, and then perform an orthogonalization step to enforce A^*A-orthogonality among a number of such spaces, say m. Like orthomin, the difference between a pair of successive approximate solutions lies in a space of low dimension, in this case k, but in the absence of arithmetic error the new approximate solution is the best in a larger space. An analysis like the one in Section 3 for orthomin would be needed to identify the selection spaces in terms of the natural oc(k, m) basis.

All implementations that rely on recursively produced, orthogonal bases can be expected to share the failing of the original conjugate gradient algorithm. The vectors are not orthogonal in practice and, as shown by Figure 1 for the conjugate gradient method, they can be quite different from the intended vectors. The loss of orthogonality in the basis is readily detected, and obviously affects the accuracy of the least squares solutions. The loss of accuracy in the basis vectors is difficult to detect, but surely affects the essential character of the approximations. Elaborate means such as reorthogonalization can remedy the orthogonality, but aside from producing more nearly orthogonal vectors, they have not been proved to result in better approximations to the underlying Krylov spaces. It is an open question whether the approximations can be made consistently better. The natural bases have been observed to be badly conditioned [7] [56], so linear transformations that make them better conditioned evidently must be ill-conditioned too, and thus must be difficult to apply accurately.

The least squares problem can be difficult to solve however it is formulated. The gcr/orthomin approach may be flawed because it solves the normal equations, but other methods must contend with near singularity of the least squares bases. The matrix H_n of the gmres approach has a 2-norm condition number no worse than A's, but by being smaller it may reflect ill-conditioning more. Alternatively, the natural bases of Krylov spaces can be very nearly singular.

It is difficult to concede that any but the best solution method should be applied to the least squares problem. For least squares problems in general, "the only fully reliable way to treat rank deficiency is to compute the singular value decomposition" [26, p. 170]. Apparently no iterative methods heed this advice. Yet the singular value decomposition is fairly inexpensive for the small matrices that appear in restarted gmres, for example, and may remove some of the difficulties occasionally reported for this method [56] [57].

In summary, existing implementations always employ orthogonal bases to reduce storage and computation. The savings in storage appear to be at most a factor of two, as for gmres versus gcr. This improvement is marginal on present-day computers and should not govern the choice of implementations. The savings in time may be more significant.

The advantages of orthogonal bases must be weighed against numerical concerns. The A^*A-orthogonal bases impose inferior least squares solution methods. In the presence of rounding error moreover, it is known that recursively generated bases may not accurately span the intended spaces. The effects of this on nonterminating, iterative algorithms are largely unexplored.

6b. An Implementation

The following implementation is generic to all oc (k, m) methods. It solves the least squares problems by the singular value decomposition, the best available method, and uses the natural bases for the Krylov spaces. This implementation is offered both as a research tool and as a model of programming simplicity. It has several advantages. First, the implementation allows easy substitution of methods, including restarted gcr/gmres and truncated orthomin. Second, it addresses some numerical difficulties likely to trouble both old and new methods. Third, it conveniently relies on well-known numerical procedures found in many scientific computing libraries. This implementation, applicable to all oc (k, m) methods and devoid of programming complications, may be the most appropriate in the present, early stages of development.

With the natural basis, all algorithms have the same implementation but for the choice of basis vectors. Methods such as conjugate residual and orthomin that don't use the full tableau can be implemented by simply choosing a subset of the larger basis. The columns of AV_n for the specific V_n of interest must be constructed explicitly. Most can be borrowed from previous steps. Only the vectors Ar_{n-1}, $A^2 r_{n-1}, \ldots, A^k r_{n-1}$ associated with the most recent solution are new. They require k matrix-vector products. The vector Ax_{n-1}, which also forms r_{n-1}, requires one more matrix-vector product or can be obtained recursively.

The least squares solution process is numerically robust. The singular value decomposition solves the least squares problem more accurately, though perhaps more expensively, than orthomin-like implementations would solve the normal equations. Errors can enter the least squares basis only through the matrix-vector multiplications which produce AV_n from V_n.

Operator coefficient methods should alleviate the concern that the natural bases for Krylov spaces are too nearly singular. High order operator coefficient methods make high degree Krylov spaces unnecessary. If very high degrees are needed, then Euclidean-orthogonal bases may be computed in the manner of Arnoldi, and may be integrated into the computations.

The following steps compute the minimum norm solution of the least squares problem. They are based on recommendations in the text of Golub and Van Loan [26]. First, the columns of AV_n should be scaled to have unit 2-norms. This makes $\kappa_2(AV_n)$ nearly minimal and improves numerical accuracy. Scaling also avoids numerical overflow and underflow when a matrix repeatedly multiplies a vector. Second, Householder transformations should reduce AV_n to an upper triangular matrix. This reduces the arithmetic costs when, as here, there are many more rows than columns. Third, the singular value decomposition of the small, upper triangular matrix must be computed. Fourth, the minimum norm solution of the column-scaled least squares problem can be approximated by applying an approximate pseudoinverse obtained by ignoring small singular values. Singular values smaller than machine round-off relative to the largest singular value might be discarded, or more sophisticated methods might be used to determine numerical rank. Finally, the unscaled minimum norm solution, c_n, combines the columns of V_n to produce the next approximate solution for the oc (k, m) method, $x_n = V_n c_n$. Table 3 restates these steps and counts their arithmetic operations.

With t basis vectors, $t \leq (k+1)m$, the implementation needs the following resources per step of the inhomogeneous oc (k, m) method. There are k matrix-vector multiplications, and one more if residuals are not recursively computed. Memory space of $2t$ vectors is needed to store V_n and the Householder transformations that

Table 3. *An implementation of oc(k, m) methods minimizing the 2-norm of the residual for a selection space basis of size $t \leq (k+1)m$, with operation counts. Terms independent of the matrix order N are omitted. Section 6b provides further explanation.*

step	operations
scale AV_n to unit column norm, $V := AV_nD^{-1}$	$3tN$
Householder transformations reduce V to triangular form, $R := QV$	$2t^2N$
orthogonal projection of y, $z := Qy$	$4tN$
singular value decomposition of R solves $\min \|RDc_n - z\|_2$	
assemble next solution, $x_n := V_nc_n$	$(2t-1)N$
optionally assemble Ax_n and r_n	$2tN$

reduce AV_n to triangular form. Very compact memory management schemes are possible since the basis vectors pass from one step to the next but the Householder transformations do not. Table 3 counts $(2t^2+9t-1)N$ arithmetic operations, from which terms independent of the matrix order, N, have been discarded. The residual calculation requires either N or $2tN$ operations.

This implementation repeatedly solves a large, dense, overdetermined, singular, least squares problem. This task is basic to numerical linear algebra. The Householder reduction and the singular value decomposition already appear in many computing libraries, and solution methods tuned to specialized computer architectures are being developed. The implementation therefore improves, in a sense automatically, with advances to numerical software and hardware.

7. Varying Coefficients

Many operator coefficient methods dynamically select recurrence coefficients by minimizing the 2-norm of the residual. This selection criterion is examined here. Theorem 1 and its Corollary prove convergence for a large class of matrices distinguished by a simple polynomial relationship. Moreover, experimental results indicate there is a trade-off between degree and order. This may allow high order methods to replace comparatively less economical high degree methods.

Theorem 1. *If the Hermitian part H of $P(A)$ is positive or negative definite for some polynomial P with degree at most k and $P(0) = 0$, then for every x_n the affine space*

$$x_n + \text{span}\left\{r_n \;\; Ar_n \;\; A^2r_n \;\; \ldots \;\; A^{k-1}r_n\right\}$$

contains a vector x_{n+1} with $\|r_{n+1}\|_2 \leq \rho \|r_n\|_2$ where

$$\rho = \sqrt{1 - \left[\frac{\min|\lambda(H)|}{\|P(A)\|_2}\right]^2} \; < \; 1.$$

The affine space also contains a vector x_{n+1}, usually different from the first, with $\|e_{n+1}\|_2 \leq \rho \|e_n\|_2$ (proof appears in Appendix 1).

Corollary to Theorem 1. *If the Hermitian part H of $P(A)$ is positive or negative definite for some polynomial P with degree at most k and $P(0) = 0$, then oc(k,m) methods whose selection spaces contain the affine space*

$$x_n + \text{span}\left\{r_n \;\; Ar_n \;\; A^2 r_n \;\; \ldots \;\; A^{k-1} r_n\right\}$$

converge for the selection criteria that minimize the 2-norm of either the residual or the error. At each step the norm declines by at least the factor

$$\sqrt{1 - \left[\frac{\min|\lambda(H)|}{\|P(A)\|_2}\right]^2} \; < \; 1.$$

The thesis of Elman [14] is the inspiration for Theorem 1. The Corollary applies to gcr$(k-1)$/gmres(k) as well as to more general methods. However, only the case in which A itself is positive or negative definite appears to have been published previously, by Eisenstat, Elman and Schultz [13]. Saad and Schultz mention this case too, and present more detailed convergence results for diagonalizable matrices [47].

Theorem 1's bound on the convergence rate may be weak because it is independent of the recurrence order m. The Theorem minimally assumes each residual r_n equals a linear combination that includes vectors from

$$\text{span}\left\{r_{n-1} \;\; Ar_{n-1} \;\; A^2 r_{n-1} \;\; \ldots \;\; A^k r_{n-1}\right\},$$

but the combination also may employ vectors from the larger space

$$\text{span}\left\{\begin{array}{cccc} r_{n-1} & r_{n-2} & \cdots & r_{n-m} \\ Ar_{n-1} & Ar_{n-2} & \cdots & Ar_{n-m} \\ \vdots & \vdots & \ddots & \vdots \\ A^k r_{n-1} & A^k r_{n-2} & \cdots & A^k r_{n-m} \end{array}\right\}.$$

Thus, r_n depends on powers of A up to A^{km}. This suggests the convergence rate may vary with the product km.

Figure 5 provides numerical evidence for this interpretation. The Figure exhibits level curves of observed convergence rates as functions of k and m for the convergence histories shown in Figure 6. The level curves have the expected qualitative behavior. In this example, the oc$(6,1)$ and oc$(3,5)$ methods have essentially the same convergence rate. This means they achieve the same accuracy in the same number of steps, but the oc$(3,5)$ method requires half the matrix-vector multiplications.

This apparent trade-off between k and m may be the most important aspect of oc(k,m) methods. It allows the beneficial effects of larger k in gcr$(k-1)$/gmres(k) to be realized more economically with larger m. The most efficient choice of k and m can be expected to change with the computer and the problem, and with the expense of solving each step's minimization problem relative to the expense of

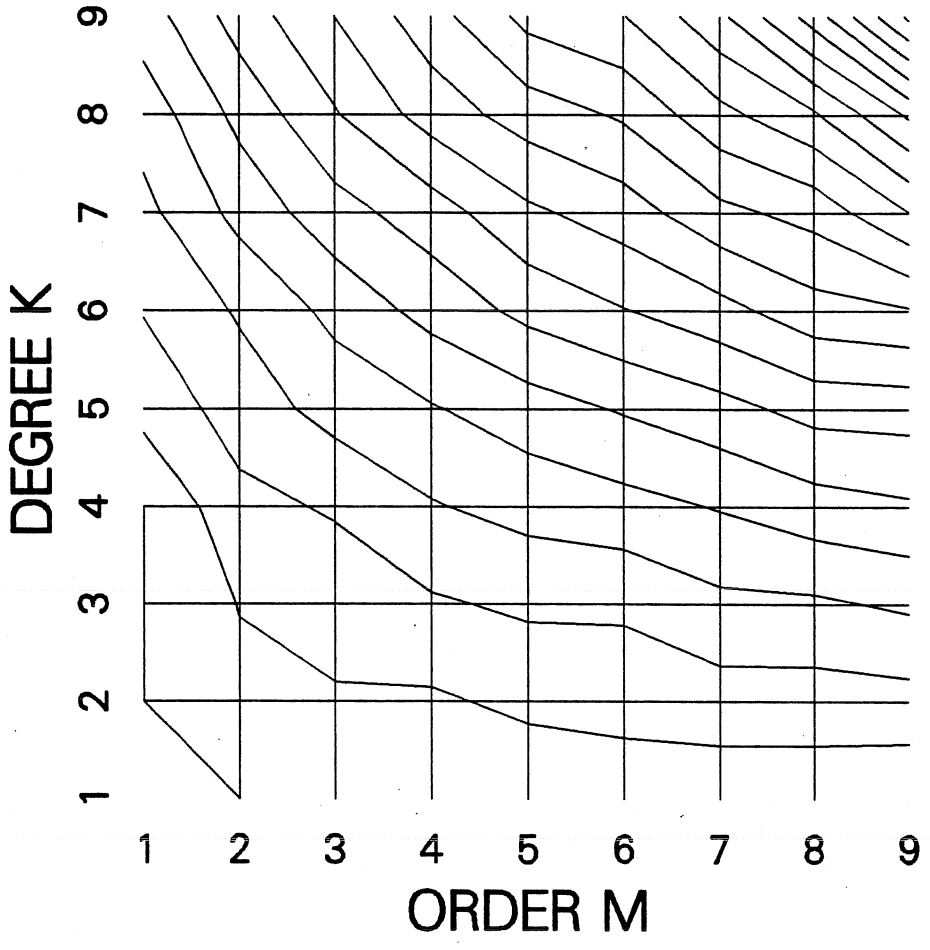

Figure 5. *Level curves of observed convergence rate for inhomogeneous* $oc(k,m)$ *as a function of* k *and* m *for one system. The curves range in multiplicative steps of* $10^{0.05}$ *from* 10^{-1} *at the upper right to* 10^{0}*, no convergence, at the lower left. The left edge corresponds to* $gcr(k-1)/gmres(k)$*, the bottom edge to* $orthomin(m-1)$*. Figure 6 displays the convergence histories. Appendix 2 and Section 7 explain the calculations.*

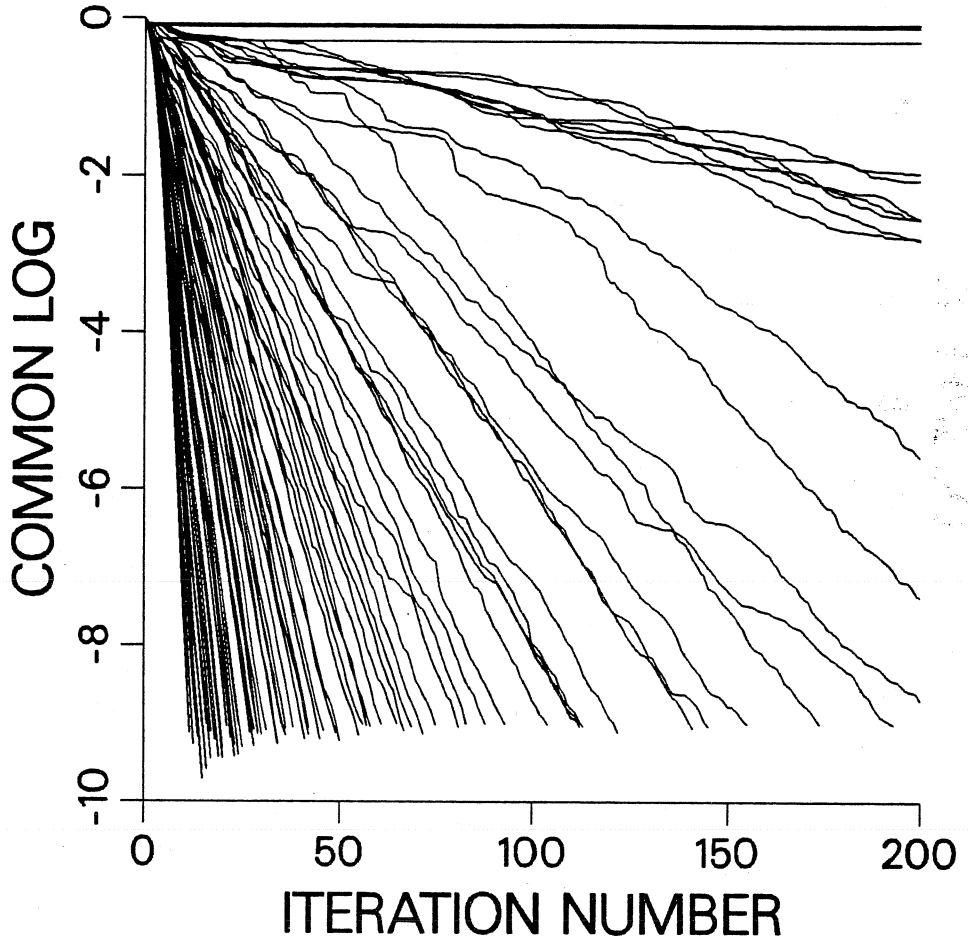

Figure 6. *Convergence histories from which the level curves of Figure 5 are derived. Appendix 2 and Section 7 explain the calculations.*

performing matrix-vector multiplications. If the convergence rate ρ did vary only with km, for example if

$$\rho(k,m) = \rho(k/\ell,\, \ell m),$$

then low degree, high order methods would be more economical. Minimizing the 2-norm of the residual involves solving a least squares problem with a basis of size $(k+1)m$ whose computation and memory requirements are roughly constant among $\mathrm{oc}(k,m)$ methods with the same km. But $\mathrm{oc}(k,m)$ performs k or $k+1$ matrix-vector multiplications per step, and this part of the total cost decreases with k. Considerations of this kind can be expected for all manner of coefficient choices.

The frequently used minimization criteria of the kind in Theorem 1 are a powerful but imprecise tool for choosing coefficients. They may not find coefficients that produce convergence, and even when they do, they may not produce the fastest convergence. Moreover, the Theorem's bound may be a poor estimate for the convergence rate because the selection criteria minimize norms of vectors, but the bound employs norms of matrices. When these matrix-vector norms are applied to matrices, they depend on both the eigenvalues and eigenvectors, while Theorem 2 in the next section shows convergence can depend on the eigenvalues alone.

The following example illustrates these concerns. The matrix

$$\begin{bmatrix} \alpha & \beta & & \\ & \alpha & \beta & \\ & & \alpha & \ddots \\ & & & \ddots \end{bmatrix}$$

has eigenvalue α and its Hermitian part has eigenvalues between $\mathrm{Real}(\alpha) \pm |\beta|$. Among $\mathrm{oc}(1,m)$ methods, a stationary Richardson's 1st order method can be made to converge independent of β, yet β can be chosen so the Hermitian part is indefinite and Theorem 1's bound is ineffective.

8. Constant Coefficients

This final section determines exactly when operator coefficient methods with constant coefficients converge. This information has several uses. First, it may guide the choice of k and m needed to achieve convergence with coefficients selected by any means. Second, it suggests ways to select coefficients other than by the usual minimization criteria of Section 7. Finally, it proves that some operator coefficient methods are new by showing they converge when previously known methods do not.

The Chebyshev iteration and the stationary 2nd order method are $\mathrm{oc}(1,2)$ methods that converge only for matrices with eigenvalues inside ellipses that exclude 0. It is demonstrated below that some constant coefficient $\mathrm{oc}(1,2)$ methods converge for non-elliptical eigenvalue distributions. These, then, are new methods.

Only the homogeneous case is possible for constant coefficients. As remarked in Section 4, with the approximate solutions converging to x_*, and with the residuals converging to 0, the sums of x-coefficients on both sides of the recurrence equation must balance.

Theorem 2. *A constant coefficient, homogeneous, operator coefficient method of degree k and order m*

$$x_n = \sum_{j=1}^{m} c_{0,j} x_{n-j} + \sum_{i=1}^{k} \sum_{j=1}^{m} c_{i,j} A^{i-1} r_{n-j}$$

with coefficient tableau

$$\begin{matrix} c_{0,1} & c_{0,2} & \cdots & c_{0,m} \\ c_{1,1} & c_{1,2} & \cdots & c_{1,m} \\ \vdots & \vdots & \ddots & \vdots \\ c_{k,1} & c_{k,2} & \cdots & c_{k,m} \end{matrix}$$

converges to a solution of $Ax = y$ for all y and all initial vectors x_0, x_{-1}, ..., x_{1-m} exactly when, for each eigenvalue λ of A, the maximum magnitude $r(\lambda)$ of the roots X of the polynomial

$$P(\lambda, X) = X^m - P_1(\lambda)X^{m-1} - P_2(\lambda)X^{m-2} - \cdots - P_m(\lambda)X^{m-m}$$

with coefficients given by the columns of the tableau

$$P_j(\lambda) = c_{0,j} - c_{1,j}\lambda - c_{2,j}\lambda^2 - \cdots - c_{k,j}\lambda^k$$

is strictly less than 1. Moreover, there is a bound upon the residuals for all y and all initial vectors x_0, x_{-1}, ..., x_{1-m}

$$\|r_n\| \leq (\|r_0\| + \|r_{-1}\| + \cdots + \|r_{1-m}\|)\, Q(n)\, R^n,$$

and if A is nonsingular there is an identical bound upon the errors

$$\|e_n\| \leq (\|e_0\| + \|e_{-1}\| + \cdots + \|e_{1-m}\|)\, Q(n)\, R^n.$$

R is the maximum $r(\lambda)$ for all the eigenvalues of A. $Q(n)$ is a polynomial that depends on the norm, on A, and on the coefficient tableau. The norm may be any consistent matrix-vector norm (proof appears in Appendix 1).

There is some evidence that constant coefficients may work well in the long run. The Chebyshev iteration's coefficients converge to values for which the stationary 2nd order method converges identically [38]. To the extent coefficients chosen by some means do become stationary, Theorem 2 explains the minimal k and m necessary before the coefficient selection criteria can make oc(k, m) methods converge. An entirely constant coefficient iteration might be useful when many systems of equations feature the same matrix. The trick is to find the coefficients, and Theorem 2 is the first step in this direction.

The following example suggests how constant coefficients might be found, and clarifies the statement of Theorem 2. Figure 7 shows that coefficients chosen to minimize the residual's 2-norm can be nearly constant over several iterations. When dynamically chosen coefficients remain fixed for a time, then a constant coefficient iteration with these fixed values may converge. To see if this is the case here, Figure 8 superimposes the matrix eigenvalues, as black dots, over some level curves of the Theorem's *eigenvalue-specific convergence rate*

$$r(\lambda) = \text{maximum } |X| \text{ of all } X \text{ for which } P(\lambda, X) = 0,$$

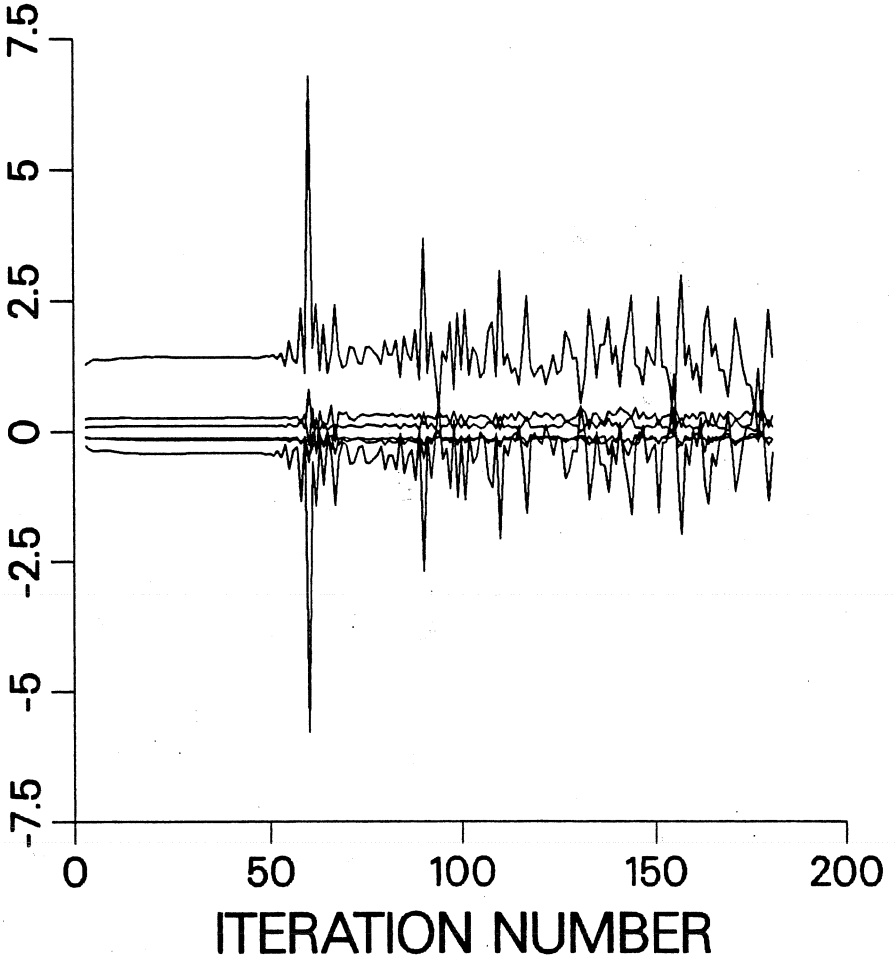

Figure 7. *Coefficients of inhomogeneous* $oc(2,2)$ *minimizing the 2-norm of the residual for one system. Appendix 2 and Section 8 explain the calculations.*

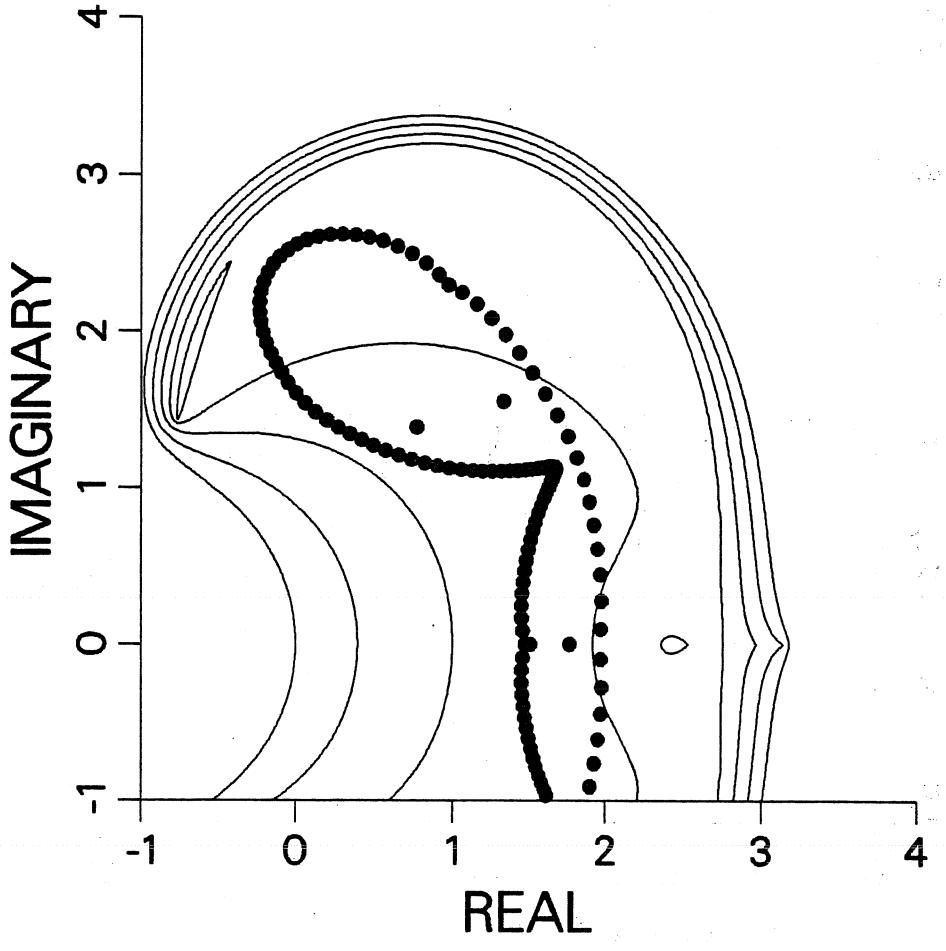

Figure 8. *Eigenvalues of the matrix (solid dots) superimposed on some level curves of the convergence rate $r(\lambda)$ for the constant coefficient regime of Figure 7. The levels start at 1 on the boundary and decrease in steps of 0.05. Appendix 2 and Section 8 explain the calculations.*

where $P(\lambda, X)$ is the Theorem's polynomial

$$P(\lambda, X) = X^m - \sum_{j=1}^{m} c_{0,j} X^{m-j} + \sum_{i=1}^{k} \sum_{j=1}^{m} c_{i,j} \lambda^i X^{m-j}$$

and where the polynomial's coefficients $c_{i,j}$ are taken from the nearly constant regime of Figure 7. The *convergence domain* is the set of λ for which $r(\lambda) < 1$. Figure 8 shows all the eigenvalues lie within the convergence domain, so Theorem 2 guarantees convergence with these constant coefficients. Figure 9 exhibits the relative residuals for the original right hand side and one other in a constant coefficient iteration.

A phenomenon discovered by Trefethen [51] explains why Figure 9 exhibits slower convergence than Figure 8 predicts. When the matrix eigenvalues are sensitive to perturbation, then convergence depends on an envelope of approximating eigenvalues introduced by rounding error. Theorem 2 must be applied to these approximations to predict the convergence rate. Nevertheless, convergence is assured in Figure 9 because a convergent iteration that already accounts for the envelope suggests the constant coefficients.

For a given matrix even with known eigenvalues or approximations thereto, it can be difficult to find any convergent coefficients let alone optimal ones that minimize Theorem 2's *convergence rate*, $R = \max r(\lambda)$. The inverse problem of finding eigenvalue domains convergent for given coefficients is at least numerically straightforward. It amounts to seeking the λ for which all the roots X of the Theorem's polynomial $P(\lambda, X)$ have magnitude less than 1.

Figure 10 displays the convergence domains for some arbitrary coefficient tableaux as large as 3×2, that is, for methods up to oc $(2, 2)$.

$$\begin{array}{ll} c_{0,1} & c_{0,2} = 1 - c_{0,1} \\ c_{1,1} & c_{1,2} \\ c_{2,1} & c_{2,2} \end{array}$$

Table 4 lists the specific coefficients.

Table 4. *Constant coefficient tableaux for the convergence domains pictured in Figure 10. Section 8 provides further explanation.*

a)	0.8	0.2	b)	0.8	0.2
	1.0	0.		1.0	−0.3
	0.	0.		0.	0.
c)	0.8	0.2	d)	1.0	0.
	1.0	−0.7		1.0	0.
	0.	0.		−0.5	0.
e)	0.8	0.2	f)	0.5	0.5
	1.0	0.		1.0	0.2
	−0.5	0.		−0.5	0.2

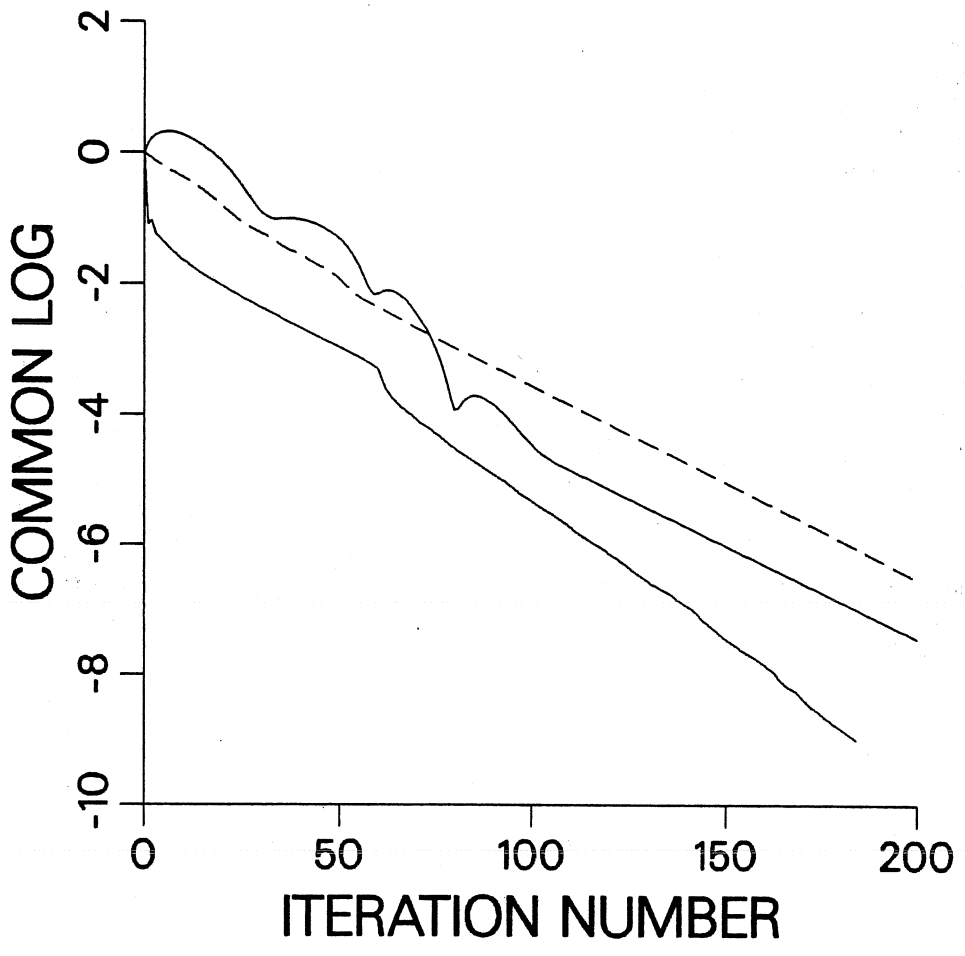

Figure 9. *2-norm relative residuals for the iteration of Figure 7 (lower solid line), and for a constant coefficient iteration with the same right hand side (higher solid line) and a different right hand side (dashed line). Appendix 2 and Section 8 explain the calculations.*

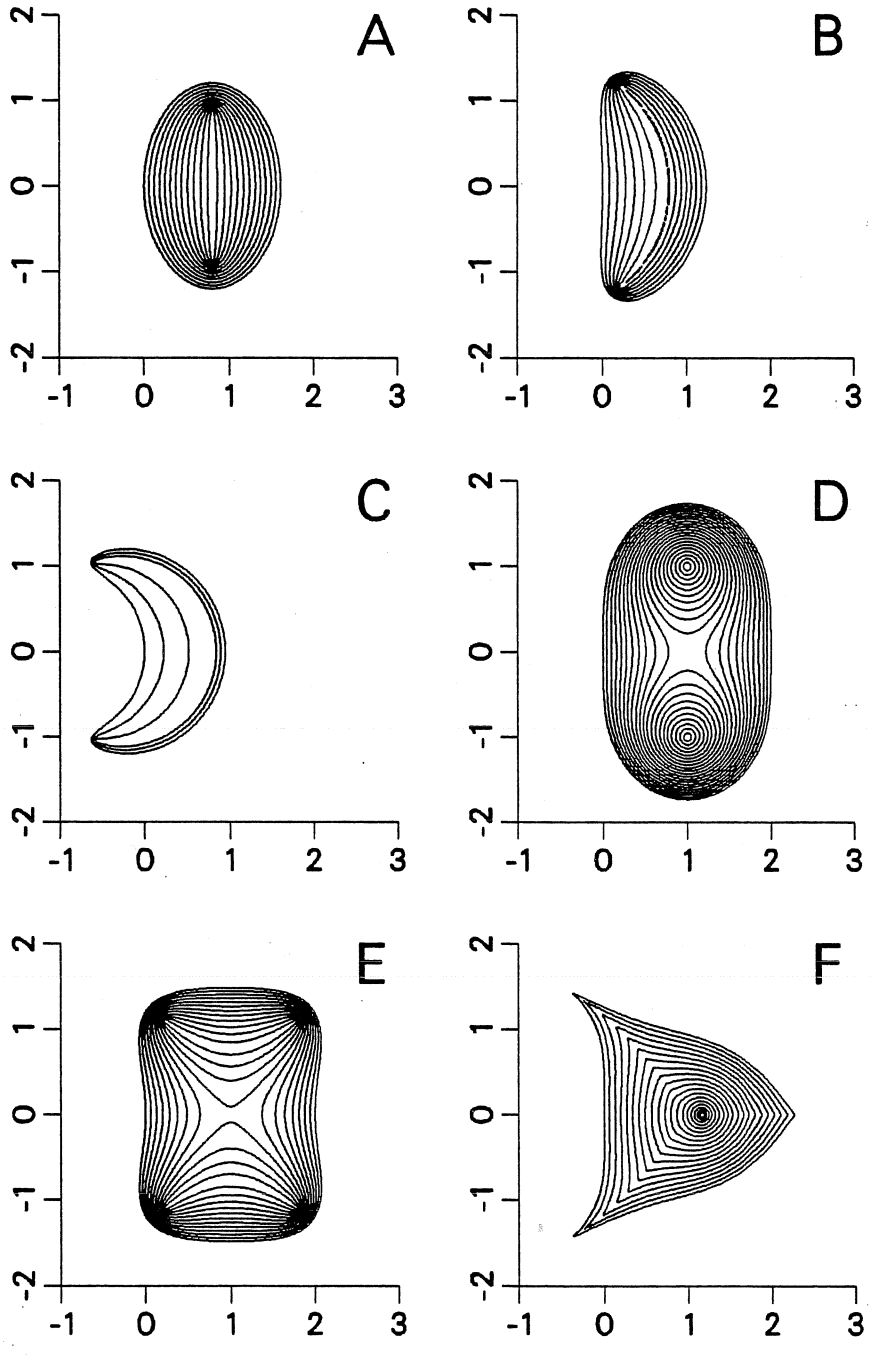

Figure 10. *Level curves of convergence rate $r(\lambda)$ as a function of λ in the complex plane for Table 4's constant coefficients. The levels begin at 1 on the boundaries and decrease in steps of 0.05. Appendix 2 and Section 8 explain the calculations.*

As explained in the survey of Section 2, Richardson's 1st order method, oc $(1,1)$, has a circular convergence domain. Figure 10a shows the typically elliptic domain of the stationary 2nd order method, oc $(1,2)$.

Figures 10b and 10c prove that some operator coefficient methods are new. Oc $(1,2)$ methods require just one matrix-vector multiplication per step, and yet fully populated 2×2 tableaux have non-elliptic convergence domains because the relationship that $P(\lambda, X) = 0$ creates between λ and X,

$$\lambda = -\frac{X^2 - c_{0,1}X - c_{0,2}}{c_{1,1}X + c_{1,2}},$$

generally does not map circles in X to ellipses in λ when $c_{1,2} \neq 0$. The domain in Figure 10b closely abuts the imaginary axis, a difficult feat for the Chebyshev iteration's ellipses. The crescent-shaped domain in Figure 10c actually crosses the axis, an impossible feat for the Chebyshev iteration's ellipses.

The remaining plots in Figure 10 illustrate the possibilities of tailoring the domain. Figure 10d is for a stationary gcr(1)/gmres(2) method, oc $(2,1)$. Figure 10e shows introducing just the previous iterate, oc $(2,2)$, produces a square convergence region. Figure 10e is for a fully populated, 3×2 tableau.

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Appendix 1. Proofs

This appendix proves the theorems cited in the text.

Theorem 1. *If the Hermitian part H of $P(A)$ is positive or negative definite for some polynomial P with degree at most k and $P(0) = 0$, then for every x_n the affine space*

$$x_n + span\left\{r_n \;\; Ar_n \;\; A^2r_n \;\; \ldots \;\; A^{k-1}r_n\right\}$$

contains a vector x_{n+1} with $\|r_{n+1}\|_2 \leq \rho \|r_n\|_2$ where

$$\rho = \sqrt{1 - \left[\frac{\min|\lambda(H)|}{\|P(A)\|_2}\right]^2} \; < \; 1.$$

The affine space also contains a vector x_{n+1}, usually different from the first, with $\|e_{n+1}\|_2 \leq \rho \|e_n\|_2$.

Proof. This proof generalizes the one Elman [14] and Eisenstat, Elman and Schultz [13] use to prove convergence of truncated orthomin. Its application in this context, and the part about minimizing the error, appear to be new.

If $r_n = 0$ then choose $x_{n+1} = x_n$. Otherwise let $P(X) = c_1X + c_2X^2 + \cdots + c_kX^k$ and choose

$$x_{n+1} = x_n + \alpha(c_1 + c_2A + \cdots + c_kA^{k-1})r_n$$

for some real α. This expression is special because $r_{n+1} = [I - \alpha P(A)]\, r_n$ so

$$\|r_{n+1}\|^2 = \|r_n\|^2 - 2\alpha r_n{}^* H r_n + \alpha^2 \|P(A)r_n\|^2.$$

Now, $\|P(A)r_n\| \neq 0$ because $P(A)r_n \neq 0$ because $r_n{}^* P(A) r_n = r_n{}^* H r_n \neq 0$ so the formula is quadratic in α. The minimum occurs at $\alpha = r_n{}^* H r_n / \|P(A)r_n\|^2$ and is

$$\|r_{n+1}\|^2 \;=\; \|r_n\|^2 - \left[\frac{r_n{}^* H r_n}{\|P(A)r_n\|}\right]^2 \;\leq\; \|r_n\|^2 - \left[\frac{\min|\lambda(H)|}{\|P(A)\|}\,\|r_n\|\right]^2.$$

There is no need to ponder the size of

$$\frac{\min|\lambda(H)|}{\|P(A)\|}.$$

It must be ≤ 1 because $\|r_{n+1}\|^2$ isn't negative. And it must be ≥ 0 because it is an absolute value over a norm. But it can't be zero because H is positive or negative definite so the numerator won't vanish.

As for minimizing the error, the choice

$$x_{n+1} = x_n + \alpha(c_1 + c_2A + \cdots + c_kA^{k-1})r_n$$

also yields $e_{n+1} = [I - \alpha P(A)]\, e_n$. This vector's norm can be minimized in the same manner as the residual's, but the minimum most likely occurs for a different α. How different? ∎

Theorem 2. *A constant coefficient, homogeneous, operator coefficient method of degree k and order m*

$$x_n = \sum_{j=1}^{m} c_{0,j} x_{n-j} + \sum_{i=1}^{k} \sum_{j=1}^{m} c_{i,j} A^{i-1} r_{n-j}$$

with coefficient tableau

$$\begin{array}{cccc} c_{0,1} & c_{0,2} & \cdots & c_{0,m} \\ c_{1,1} & c_{1,2} & \cdots & c_{1,m} \\ \vdots & \vdots & \ddots & \vdots \\ c_{k,1} & c_{k,2} & \cdots & c_{k,m} \end{array}$$

converges to a solution of $Ax = y$ for all y and all initial vectors x_0, x_{-1}, ..., x_{1-m} exactly when, for each eigenvalue λ of A, the maximum magnitude $r(\lambda)$ of the roots X of the polynomial

$$P(\lambda, X) = X^m - P_1(\lambda)X^{m-1} - P_2(\lambda)X^{m-2} - \cdots - P_m(\lambda)X^{m-m}$$

with coefficients given by the columns of the tableau

$$P_j(\lambda) = c_{0,j} - c_{1,j}\lambda - c_{2,j}\lambda^2 - \cdots - c_{k,j}\lambda^k$$

is strictly less than 1. Moreover, there is a bound upon the residuals for all y and all initial vectors x_0, x_{-1}, ..., x_{1-m}

$$\|r_n\| \leq (\|r_0\| + \|r_{-1}\| + \cdots + \|r_{1-m}\|)\, Q(n)\, R^n,$$

and if A is nonsingular there is an identical bound upon the errors

$$\|e_n\| \leq (\|e_0\| + \|e_{-1}\| + \cdots + \|e_{1-m}\|)\, Q(n)\, R^n.$$

R is the maximum $r(\lambda)$ for all the eigenvalues of A. $Q(n)$ is a polynomial that depends on the norm, on A, and on the coefficient tableau. The norm may be any consistent matrix-vector norm.

Proof. The Theorem is not trivial because it allows defective A, but the proof's main challenges are notation and pruning. There are nine parts.

Part 1. Much of what is needed to prove the Theorem can be taken from the literature of finite differences [39]. The proof depends on sequences $\{\tau_n\}$ generated by constant coefficient, homogeneous, m^{th} order, linear recurrence formulas

$$\tau_n = \sum_{j=1}^{m} P_j \tau_{n-j}.$$

The sequences begin from initial values τ_0, τ_{-1}, ..., τ_{1-m} and the formulas apply when $n \geq 1$. Any recurrence sequence can be expressed as a linear combination of *fundamental sequences* of the form $\{n^{i-1}\rho^n\}$ in which ρ is a root of multiplicity at least i of the *characteristic polynomial*

$$X^m - \sum_{j=1}^{m} P_j X^{m-j}.$$

The coefficients in the linear combination for $\{\tau_n\}$ can be obtained by solving an $m \times m$ system of linear equations. Each column of the coefficient matrix M contains the initial values of a different fundamental sequence, and the column on the right side of the equations contains the initial values of $\{\tau_n\}$. This formula for the coefficients leads to the following bound

$$|\tau_n| \leq n^{m-1} r^n \|M^{-1}\|_1 \sum_{j=1}^{m} |\tau_{1-j}|$$

in which $n \geq 1$ and r is the magnitude of the largest root ρ. The power n^{m-1} only occurs in the worst case when the characteristic polynomial has a single root of multiplicity m.

The bound is needed for recurrence sequences whose coefficients P_j are polynomials of a parameter λ. In this case, the characteristic polynomial is the $P(\lambda, X)$ in the statement of the Theorem. A technical detail occurs when P_m vanishes for some λ, because then the recurrence has order less than m. The bound remains valid for a smaller matrix M and a smaller order m, but it is notationally convenient to retain the original m. Thus, for specific polynomials $P_j(\lambda)$ there is a bound

$$|\tau_n| \leq n^{m-1} r(\lambda)^n q(\lambda) \sum_{j=1}^{m} |\tau_{1-j}|$$

in which $r(\lambda)$ is the magnitude of the largest root of the characteristic polynomial, and $q(\lambda)$ is a number with a rather complicated definition. The $r(\lambda)$ and $q(\lambda)$ depend on the recurrence coefficients, that is, on the coefficient tableau of the operator coefficient method.

Part 2. The recurrence formulas generate another collection of fundamental sequences, here denoted $\{\pi_{n,k}\}$ for k from 1 to m. These sequences have only one nonzero initial value apiece, namely $\pi_{1-k,k} = 1$ and others 0. When they represent any other recurrence sequence in the manner of Part 1, then the coefficients in the linear combination are just the other's initial values.

$$\tau_n = \sum_{k=1}^{m} \tau_{1-k} \pi_{n,k}$$

In this way a homogeneous sequence has a closed-form representation terms of its initial values.

Part 3. Adding an extra term σ_ℓ to τ_ℓ amounts to beginning a new recurrence sequence with initial value σ_ℓ. The contribution to $\tau_{\ell+1}$ is $\pi_{1,1}\sigma_\ell$, the contribution to $\tau_{\ell+2}$ is $\pi_{2,1}\sigma_\ell$, and so on. The sequence of multipliers is $\{\pi_{n,1}\}$. One sequence suffices independent of ℓ because the recurrence formulas have constant coefficients. In combination with Part 2 therefore, a nonhomogeneous recurrence

$$\tau_n = \sigma_n + \sum_{j=1}^{m} P_j \tau_{n-j}$$

has a closed-form representation

$$\tau_n = \sum_{\ell=1}^{n} \pi_{n-\ell,1} \sigma_\ell + \sum_{k=1}^{m} \pi_{n,k} \tau_{1-k}.$$

Part 4. When the recurrence coefficients $P_1, P_2, \ldots, P_m$ are polynomials of λ as they are here, then so are the $\pi_{n,k}$'s. Their recurrence formula

$$\pi_{n,k} = \sum_{j=1}^{m} P_j \pi_{n-j,k}$$

can be differentiated s times

$$\begin{aligned}\pi_{n,k}^{(s)} &= \sum_{i=0}^{s}\sum_{j=1}^{m} \binom{s}{i} P_j^{(i)} \pi_{n-j,k}^{(s-i)} \\ &= \sum_{j=1}^{m} P_j \pi_{n-j,k}^{(s)} + \sum_{i=1}^{s}\sum_{j=1}^{m} \binom{s}{i} P_j^{(i)} \pi_{n-j,k}^{(s-i)}\end{aligned}$$

to reveal that the derivatives satisfy nonhomogeneous recurrence formulas. The superscripts in parentheses denote derivatives of various orders with respect to λ. The derivative sequences have zeroes for initial values, that is, only the nonhomogeneous terms participate in Part 3's closed-form expansion.

$$\pi_{n,j}^{(s)} = \sum_{\ell=1}^{n}\sum_{i=1}^{s}\sum_{j=1}^{m} \binom{s}{i} \pi_{n-\ell,1} P_j^{(i)} \pi_{n-j,k}^{(s-i)}$$

This represents each derivative entirely in terms of lower-order derivatives.

Part 5. The bounds of Part 1 can be applied first to the polynomials $\pi_{n,k}$ of Part 2 and then to the derivative formulas of Part 5 to obtain

$$\left|\pi_{n,k}^{(s)}(\lambda)\right| \le q_s(n,\lambda)\, r(\lambda)^n$$

where q_s is a polynomial of n. Part 1 forces the choice

$$q_0(n,\lambda) = n^{m-1} q(\lambda),$$

and the others can be constructed recursively by

$$q_s(n,\lambda) = n\, q_0(n,\lambda)\, q_{s-1}(n,\lambda)\, m\, 2^s \max_{1\le i\le s,\ 1\le j\le m} \left|P_j^{(i)}(\lambda)\right|.$$

Only the polynomial dependence on n is important. The bounds aren't sharp and needn't be. They have been chosen to increase monotonically with n and s to ease the following derivation.

$$\begin{aligned}\left|\pi_{n,k}^{(s)}(\lambda)\right| &= \left|\sum_{\ell=1}^{n}\sum_{i=1}^{s}\sum_{j=1}^{m} \binom{s}{i} \pi_{n-\ell,1}(\lambda) P_j^{(i)}(\lambda) \pi_{n-j,k}^{(s-i)}(\lambda)\right| \\ &\le \sum_{\ell=1}^{n}\sum_{i=1}^{s}\sum_{j=1}^{m} \binom{s}{i} q_0(n,\lambda) \left|P_j^{(i)}(\lambda)\right| q_{s-1}(n,\lambda) \\ &\le n\, q_0(n,\lambda)\, q_{s-1}(n,\lambda) \sum_{i=1}^{s}\sum_{j=1}^{m} \binom{s}{i} \left|P_j^{(i)}(\lambda)\right| \\ &\le q_s(n,\lambda)\end{aligned}$$

Part 6. At this point its customary to cite an unimpeachable source for the definition and existence of a Jordan decomposition, $J = UAU^{-1}$. This allows individual Jordan blocks to be considered. Manteuffel [35] [36] observes that evaluating a polynomial $\pi(X)$ at a Jordan block amounts to differentiating the polynomial. If λ is the block's eigenvalue, there results an upper triangular, Toeplitz matrix with $\pi^{(i)}(\lambda)/i!$ on the i^{th} superdiagonal, as in the example below.

$$\pi\left(\begin{bmatrix} \lambda & 1 & \\ & \lambda & 1 \\ & & \lambda \end{bmatrix}\right) = \begin{bmatrix} \pi^{(0)}(\lambda)/0! & \pi^{(1)}(\lambda)/1! & \pi^{(2)}(\lambda)/2! \\ & \pi^{(0)}(\lambda)/0! & \pi^{(1)}(\lambda)/1! \\ & & \pi^{(0)}(\lambda)/0! \end{bmatrix}$$

In this way the bounds of Part 5 can be applied to each Jordan block and then combined for all blocks to obtain bounds

$$\|\pi_{n,k}(A)\| = \|U^{-1}\pi_{n,k}(J)\,U\| \leq Q(n)R^n.$$

R is the largest $r(\lambda)$ for all the matrix eigenvalues. $Q(n)$ is a polynomial that depends on the norm, on A, and on the coefficient tableau. The norm should be a consistent matrix-vector norm because the next step applies it to both.

Part 7. Remembering the original use of the $\pi_{n,k}$'s in Part 2 and the bounds in Part 6, the terms of vector sequences $\{t_n\}$ generated from initial values $t_0, t_{-1}, \ldots, t_{1-m}$ by a constant coefficient, homogeneous, m^{th} order, linear recurrence formula

$$t_n = \sum_{j=1}^{m} P_j(A)t_{n-j},$$

whose coefficients are polynomials of A, are expressed by

$$t_n = \sum_{k=1}^{m} \pi_{n,k}(A)t_{1-k}$$

and are bound by

$$\|t_n\| \;\leq\; Q(n)R^n \sum_{k=1}^{m} \|t_{1-k}\|.$$

Part 8. The preliminaries are finished and the theorem's proof begins here. Since the operator coefficient method is homogeneous there is a residual recurrence

$$r_n = \sum_{j=1}^{m} P_j(A)r_{n-j}$$

and if A is nonsingular this can be multiplied by A^{-1} to obtain an error recurrence

$$e_n = \sum_{j=1}^{m} P_j(A)e_{n-j}$$

and from Part 7 both sequences satisfy the bounds in the statement of the Theorem.

Part 9. If A is singular then the Theorem's polynomial for $\lambda = 0$ is

$$P(0, X) = X^m - c_{0,1}X^{m-1} - c_{0,2}X^{m-2} - \cdots - c_{0,m}X^{m-m}$$

which has 1 as a root because $c_{0,1} + c_{0,2} + \cdots + c_{0,m} = 0$ in the homogeneous case, so $1 = r(0) \leq R$. Thus, if $R < 1$ then 0 is not an eigenvalue, A is nonsingular, and a solution exists. The bound in Part 8 shows the errors converge to zero since

$$\lim_n Q(n)R^n = 0$$

whenever Q is a polynomial of n. The Theorem's convergence criterion is therefore sufficient. If $1 \leq R$, then from the Jordan block of the eigenvalue for which the Theorem's polynomial has a root of magnitude R, it is possible to construct some y and initial vectors $x_0, x_{-1}, \ldots, x_{1-m}$ so the corresponding residuals satisfy $\|r_n\| = \|r_0\|R^n$. The Theorem's convergence criterion therefore is necessary. ∎

Appendix 2. Figure Explanations

This appendix explains the numerical experiments reported in the Figures. All calculations are performed by a Cray XMP with unit roundoff 3.5×10^{-15}. The initial guess x_0 for all iterations is 0.

Figure 1. *2-norm relative errors in the computed basis vectors of the conjugate gradient algorithm for a system of order* 100.

Figure 2. *Relative A-norm solution errors for the system of Figure 1. The upper curve is for single precision and the lower for reorthogonalized double precision.*

For Figures 1 and 2 the system $Ax = y$ has diagonal A with entries 1^2, 2^2, ..., 100^2 and uniform y with entries 1, 1, ..., 1. The single precision conjugate gradient algorithm appears in Section 2 and has explicit, not recursive, residuals. Its deviation from what would be obtained from exact, infinite precision calculations is measured by comparison with a double precision version that includes full orthogonalization in which

$$p_n = r_n - \sum_{j=1}^{n} \frac{{p_{n-j}}^* A r_n}{{p_{n-j}}^* A p_{n-j}} p_{n-j}$$

replaces

$$p_n = r_n - \frac{{p_{n-1}}^* A r_n}{{p_{n-1}}^* A p_{n-1}} p_{n-1}.$$

Figure 1 actually plots $\|p_n^{(1)} - p_n^{(2)}\|_2 / \|p_n^{(2)}\|_2$ and Figure 2 plots both $\|e_n^{(1)}\|_A / \|x_*\|_A$ and $\|e_n^{(2)}\|_A / \|x_*\|_A$. The superscripts distinguish single and double precision values.

Figure 3. *2-norm relative residuals for homogeneous (dashed) and inhomogeneous (solid) gcr(k−1)/gmres(k), k = 1, 2, ..., 10, applied to one system. The two methods perform alike except for $k = 5$ when the original, homogeneous method stagnates and the new, inhomogeneous method converges.*

For Figures 3, 4, 5 and 6 the system $Ax = y$ resembles one used by Elman and Streit [15]. The matrix is a preconditioned discretization of

$$\left(-\frac{\partial^2}{\partial x \partial y} + \alpha \frac{\partial}{\partial x} + \beta \frac{\partial}{\partial y} - \gamma \right) u = f$$

for real-valued u on $[0,1] \times [0,1]$ with zero Dirichlet boundary data. The finite difference discretization has a 33×33 uniform grid with 961 interior unknowns related by 5-point approximations to second derivatives and by centered approximations to first derivatives. The preconditioned system is $A_2^{-1} A_1 x = y$ where A_1 is the discrete operator for $\alpha = 50$, $\beta = 100$, $\gamma = 250$ and where A_2 is the discrete operator for $\alpha = \beta = \gamma = 0$. A stabilized block cyclic reduction method performs the multiplication by A_2^{-1} [26]. The entries of y are uniformly and randomly distributed between -1 and 1.

Gcr($k-1$)/gmres(k) is implemented in the simplest possible manner suggested by Table 1. The singular value decomposition solves the least squares problem

$$\text{minimize } \|r_{n+1}\| \text{ over } x_n + \text{span}\left\{r_n \;\; Ar_n \;\; A^2r_n \;\; \ldots \;\; A^{k-1}r_n\right\}$$

by projecting r_n into span $\left\{Ar_n \;\; A^2r_n \;\; \ldots \;\; A^kr_n\right\}$. The inhomogeneous version solves

$$\text{minimize } \|r_{n+1}\| \text{ over span } \left\{x_n \;\; r_n \;\; Ar_n \;\; A^2r_n \;\; \ldots \;\; A^{k-1}r_n\right\}$$

by projecting y into span $\left\{Ax_n \;\; Ar_n \;\; A^2r_n \;\; \ldots \;\; A^kr_n\right\}$.

Figure 4. *2-norm relative residuals for homogeneous (dashed) gcr(5)/gmres(6) and inhomogeneous (solid) oc$(6,m)$, $m = 1\ 2 \ldots 10$, applied to the same system.*

The system of equations and the implementation of homogeneous gcr($k-1$)/gmres(k) are described with Figure 3. The implementation of the inhomogeneous oc(k,m) methods is described in Section 6b. When $m = 1$ it is identical to Figure 3's inhomogeneous gcr($k-1$)/gmres(k).

Figure 5. *Level curves of observed convergence rate for inhomogeneous oc(k,m) as a function of k and m for one system. The curves range in multiplicative steps of $10^{0.05}$ from 10^{-1} at the upper right to 10^0, no convergence, at the lower left. The left edge corresponds to gcr($k-1$)/gmres(k), the bottom edge to orthomin($m-1$). Figure 6 displays the convergence histories. Figure 6 displays the convergence histories.*

Figure 6. *Convergence histories from which the level curves of Figure 5 are derived.*

The system of equations is the one for Figures 3 and 4. Section 6b describes the implementation of the inhomogeneous oc(k,m) methods. Least squares linear fits to the last half of each curve in Figure 6's logarithmic scale produce the observed convergence rates. The level curves are obtained by extending the fits to the logarithmic data bilinearly throughout the cells of the $k \times m$ grid.

Figure 7. *Coefficients of inhomogeneous oc$(2,2)$ minimizing the 2-norm of the residual for one system.*

Figure 8. *Eigenvalues of the matrix (solid dots) superimposed on some level curves of the convergence rate $r(\lambda)$ for the constant coefficient regime of Figure 7. The levels start at 1 on the boundary and decrease in steps of 0.05.*

Figure 9. *2-norm relative residuals for the iteration of Figure 7 (lower solid line), and for a constant coefficient iteration with the same right hand side (higher solid line) and a different right hand side (dashed line).*

For Figures 7, 8 and 9 the matrix is Toeplitz and banded with -1's on the first superdiagonal and with 1's on the main and first 3 subdiagonals. Careless programming resulted in a matrix of order 201. For Figure 7 the entries of the right side all equal 1. The implementation of the inhomogeneous oc$(2,2)$ method is

described in Section 6b. Figure 7 plots the 6 coefficients in the 3×2 tableaux. The coefficients for the first few tableaux are not shown because they are larger than the others. The coefficients for the next several iterations vary on the order of one percent from

$$\begin{array}{rr} 1.421 & -0.421 \\ 0.261 & -0.172 \\ -0.130 & 0.102 \end{array}$$

which are the constant coefficients used for Figures 8 and 9. These Figures are explained by their captions and by Section 8. The other right hand side for Figure 9 has entries uniformly and randomly distributed between -1 and 1.

Figure 10. *Level curves of convergence rate $r(\lambda)$ as a function of λ in the complex plane for Table 4's constant coefficients. The levels begin at* 1 *on the boundaries and decrease in steps of* 0.05.

Like Figure 8, the curves are formed by plotting the contours of

$$r(\lambda) = \text{maximum } |X| \text{ of all } X \text{ for which } P(\lambda, X) = 0$$

using the quadratic formula to solve $P(\lambda, X) = 0$ when $m = 2$.

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