ON THE CONVERGENCE RATE OF A PRECONDITIONED SUBSPACE EIGENSOLVER[1]

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Abstract. In this paper we present a proof of convergence for a preconditioned subspace method which shows the dependency of the convergence rate on the preconditioner used. This convergence rate depends only on the condition of the pre-conditioned system $\kappa_2(MA)$ and the relative separation of the first two eigenvalues $1 - \lambda_1/\lambda_2$. This means that, for example, multigrid preconditioners can be used to find eigenvalues of elliptic PDE's at a grid-independent rate.

KEYWORDS: eigenvalue problems, convergence rate, Generalized Davidson
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1. Introduction.

Jacobi–Davidson type algorithms have received a lot of attention lately. Sleijpen and Van der Vorst's paper [16] provides illuminating insights into the understanding of this class of algorithms and on the use of preconditioners within these methods. The original Davidson algorithm used a diagonal preconditioner [6]. This was later extended to allow for a general preconditioner (Generalized Davidson) [15]. Assume that we are searching for the smallest eigenvalue λ_1 of A and let $\widehat{\lambda}_k$ denote the k^{th} iterative approximation to λ_1. Newton type eigensolvers solve the following equation

$$(A - \widehat{\lambda}_k I)t = \epsilon u_k - r, t \perp u_k, \tag{1.1}$$

where u_k and $\widehat{\lambda}_k$ are current guesses for the eigenpair and r is the current residual. This is the basis of the method presented in Olsen, Jorgensen and Simon [13]. In its original formulation the Generalized Davidson algorithm solves $(A - \widehat{\lambda}_k I)t = r$ approximately and then orthogonalizes t with respect to span V_k. So the use of a preconditioner to approximate the inverse of $(A - \widehat{\lambda}_k I)$ seems highly desirable. Some problems with a preconditioner in this context [18, 17] are: I) When $(A - \widehat{\lambda}_k I)^{-1}$ is approximated well you get $t = u_k$ (the current eigenvector approximation). II) If $\widehat{\lambda}_k$ is close to an exact eigenvalue, $(A - \widehat{\lambda}_k I)$ is ill-conditioned. III) $(A - \widehat{\lambda}_k I)$ is indefinite if $\widehat{\lambda}_k$ is not an extreme eigenvalue. IV) misconvergence. V) complex eigenvalues of real matrices leads to a complex preconditioner, which is more expensive computationally.

The Jacobi–Davidson method [16] explicitly overcomes some of these problems, by replacing (1.1) with

$$(I - u_k u_k^*)(A - \widehat{\lambda}_k I)(I - u_k u_k^*)t = -r \tag{1.2}$$

where u_k is the current eigenvector approximation, and using a preconditioner for this system instead. The solution and right hand side of (1.2) are understood to be orthogonal to u_k. In this method, stalling problems are avoided (I), and the conditioning of the equations is better when the eigenvalue is simple (II). Sleijpen and Van der Vorst [16] give some examples of problems for which the Jacobi–Davidson method performs much better than when $M_k = (A - \widehat{\lambda}_k I)^{-1}$ is used in the Generalized Davidson method. The explanation for the difference in performance appears to rest on the

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fact that the preconditioner which approximates $(A-\widehat{\lambda}_k I)^{-1}$ is unbounded as $k \to \infty$, for $\widehat{\lambda}_k$ approaching a simple eigenvalue λ_1, while $[(I-u_k u_k^T)(A-\widehat{\lambda}_k I)(I-u_k u_k^T)]^+$ is bounded as $k \to \infty$.

Since the Jacobi–Davidson method solves the system on the space orthogonal to u_k (see (2)), the chosen preconditioner for Jacobi–Davidson only needs to be defined on this restricted subspace. A consequence of the formulation (1.2) is that the Jacobi–Davidson preconditioner belongs to a set which is a restriction of all the possible preconditioners allowed by the Generalized Davidson (GD) algorithm.

Another way to overcome (II) is to use a fixed preconditioner with the GD algorithm and analyse its convergence behavior. In this paper, we show that if a fixed preconditioner M (independent of $\widehat{\lambda}_k$) is used, we can get rapid linear convergence with the Generalized Davidson algorithm, as is the case for the Jacobi–Davidson method. Previous numerical results from the author [12] indicate that preconditioners for the Generalized Davidson algorithm which are independent of $\widehat{\lambda}_k$ work well, at least for some PDE problems. The theoretical development of this paper presents results for preconditioners which are independent of $\widehat{\lambda}_k$. Examples of these preconditioners are the same used for solution of positive definite systems of equations, such as incomplete factorization [9], multigrid, or domain decomposition preconditioners [8, 7]. In the case of multigrid preconditioners, the cost is $O(N)$ for each preconditioning step.

Some papers [14, 16] have noted that if the preconditioner is $(A-\widehat{\lambda}_k I)^{-1}$, then superlinear convergence can be obtained for inverse iteration and the Jacobi–Davidson method. However, this requires the use of specialized solvers to accurately solve indefinite problems, which are considerably more complex than solvers for positive definite problems. These indefinite solvers are themselves typically linearly convergent iterative methods, and consequently convergence is slow in terms of the error reduction for a fixed amount of computational work. Some papers have dealt with convergence proofs for Richardson-type eigensolvers [4]. This other class of preconditioned eigensolvers [4] is not related to Jacobi–Davidson or Generalized Davidson algorithms.

In this paper we will develop a bound on the rate of convergence for Davidson type algorithms in terms of the condition number $\kappa_2(MA)$ of the preconditioned system, and the relative gap for the desired eigenvalue $1-\lambda_1/\lambda_2$ where λ_2 is the second *distinct* eigenvalue of A. The bounds obtained here are similar to the traditional bounds for convergence rates for preconditioned systems of linear equations. For example, if we use multigrid preconditioned conjugate gradient algorithms for suitable discretizations of elliptic PDE's (with smooth coefficients) the convergence rate can be shown to be bounded independently of the grid spacing. This is because for a multigrid preconditioner M, the condition number $\kappa_2(MA)$ can be bounded independently of the grid spacing for these equations. We will show that if we use the same preconditioner for GD algorithms, the convergence of the eigenvalue solver is also grid independent. The only assumptions used in this paper are bounded $\kappa_2(MA)$, and that A and M are symmetric positive definite matrices. The remainder of the paper goes as follows: in Section 2 we review the Generalized Davidson algorithm; a bound on the rate of convergence for GD is presented in Section 3. Section 4 relates the results of Section 3 to the condition number of the preconditioned system. In Section 5 we summarize the main results of this paper.

2. Generalized Davidson Algorithm. The Generalized Davidson algorithm involves the computation of an orthonormal basis for a subspace from a given starting vector x_0. This subspace depends on a preconditioner applied to the current residual.

In other words, the GD algorithm generates an orthonormal basis $\{ v_0, v_1, \ldots, v_{k-1} \}$ for subspaces which depend on A, x_0 and the M_λ matrices. From these orthonormal bases, projected matrices are computed $S_k = V_k^T A V_k$, which are usually dense, making the calculation of eigenvalues on the subspace more expensive than it is for the Lanczos algorithm. Nevertheless, the preconditioning step in this algorithm can reduce the total number of iterations considerably, giving a more attractive subspace algorithm overall. An example of a method belonging to this class is the Jacobi-Davidson method presented in [16]. The Generalized Davidson algorithm with preconditioner M_λ proceeds as shown in Algorithm 1.

ALGORITHM 1. – ***Generalized Davidson Algorithm***

Given an initial vector $x_1 \neq 0$ and iteration limit m, eigenvalue number p, and convergence tolerance ϵ, compute V_k, S_k, $\widehat{\lambda}_k$ and u_k.

1. Set $v_1 \leftarrow x_1/\|x_1\|_2$.
2. $V_1 \leftarrow [v_1]$; $W_0 \leftarrow [\,]$.
3. **for** $k = 1, \ldots, m$ **do**...
   (a) $w_k \leftarrow A v_k$.
   (b) $W_k = [W_{k-1}, w_k]$.
   (c) Compute $V_k^T w_k$ and make it the last column & row of $S_k = V_k^T A V_k = V_k^T W_k$.
   (d) $\ell \leftarrow \min(k, p)$
   (e) Compute the ℓth smallest eigenpair $\widehat{\lambda}_k$, y_k of S_k: $S_k y_k = \widehat{\lambda}_k y_k$, $y_k \neq 0$. (This can be done using the QR algorithm.)
   (f) $u_k \leftarrow V_k y_k$ (Ritz vector).
   (g) $r_k \leftarrow A u_k - \widehat{\lambda}_k u_k = W_k y_k - \widehat{\lambda}_k V_k y_k$ (residual vector).
   (h) If $\|r_k\|_2 < \epsilon$ then exit loop.
   (i) If $k < m$
      - $t_k \leftarrow M_{\widehat{\lambda}_k} r_k$.
      - $v_{k+1} \leftarrow mgs(V_k, t_k)$ where $mgs(V_k, t_k)$ is the result of applying the modified Gram–Schmidt process to orthonormalize t against the columns of V_k.
      - $V_{k+1} \leftarrow [V_k, v_{k+1}]$

Note that this algorithm does not necessarily represent the original matrix on a Krylov subspace. Instead, the original matrix A is represented in a subspace span V_k which is constructed with an initial vector v_1 and subsequent preconditioned residuals $(M_{\widehat{\lambda}_k} r_k)$. The theoretical development in [5] has shown that where the largest (smallest) eigenvalue is sought, and the preconditioning matrices are uniformly bounded and uniformly positive definite, then the largest (smallest) eigenvalue $\widehat{\lambda}_k$ of S_k converges to an eigenvalue of A as $k \to \infty$, and that the associated eigenvectors for the eigenvalues $\widehat{\lambda}_k$ converge to eigenvectors of A. As noted in Section 1, this paper results are for preconditioners $M_{\widehat{\lambda}_k} = M$ which are independent of $\widehat{\lambda}_k$.

In practice, for certain quantum chemistry calculations, the GD algorithm has been shown to be very efficient, requiring a small number of iterations to compute the smallest or largest eigenvalue and eigenvector pairs for matrices of sizes 10^3 to 10^5 and even 10^6. This is because, for these applications, the matrices considered were strongly diagonally dominant, and the choice of the preconditioner $M_{\widehat{\lambda}_k} = (D - \widehat{\lambda}_k I)^{-1}$ with $D = \text{diag}(A)$ gives very good convergence rates. However, for matrices obtained from PDE's, the use of this preconditioner gives no significant improvement over Lanczos.

Thus the speed obtained for the GD algorithm depends crucially on the nature of the preconditioners involved. If poor preconditioners are used, then this method gives little or no improvement on the Lanczos algorithm. If an exact inverse $M_{\widehat{\lambda}_k} = (A - \widehat{\lambda}_k I)^{-1}$ is used with the Davidson algorithm it leads to stagnation, while with the Jacobi-Davidson algorithm it leads to cubic convergence [16].

3. Rate of Convergence for the Generalized Davidson Algorithm with Fixed Preconditioner. A proof of convergence of the Generalized Davidson algorithm is given in Crouzeix, Philippe and Sadkane [5]. However, they do not obtain any estimates of the *rate of convergence*, or explain its dependence on the preconditioner chosen. This is an important issue, since the performance of the Generalized Davidson algorithm is crucially dependent on the preconditioner.

Let A be the given matrix whose eigenvalues and eigenvectors are sought. The preconditioner M is given for one step, and Davidson's algorithm is used with u_k being the current computed approximate eigenvector. The current eigenvalue estimate is the Rayleigh quotient $\widehat{\lambda}_k = \rho_A(u_k) = (u_k^T A u_k)/(u_k^T u_k)$. Let the exact eigenvector with the smallest eigenvalue of A be u, and

$$Au = \lambda_1 u.$$

(If λ_1 is a repeated eigenvalue of A, then we can let u be the normalized projection of u_k onto this eigenspace.)

THEOREM 3.1. *Let P be the orthogonal projection onto $ker(A - \lambda_1 I)^{\perp}$. Suppose that A and M are symmetric positive definite and $M_{\widehat{\lambda}} = M$ is fixed. If $\gamma > 0$ and*

$$\sigma = \|P - \gamma(A - \lambda_1 I)^{1/2} PMP (A - \lambda_1 I)^{1/2}\|_2 < 1,$$

then for almost any starting value x_1, the eigenvalue estimates $\widehat{\lambda}_k$ converge to λ_1 ultimately geometrically with convergence factor bounded by σ^2, and the angle between the exact and computed eigenvector goes to zero ultimately geometrically with convergence factor bounded by σ.

Proof. The proof of convergence in [5] applies under the hypotheses of this theorem and shows that the method converges. Here we show a bound on the convergence rate under the assumptions above. Therefore we can assume that k is "sufficiently large" and that $u_k = \alpha_k u + \beta_k s_k$ with β_k "sufficiently small". Set $\|u_k\|_2 = \|u\|_2 = \|s_k\|_2 = 1$ and $s_k \perp u$, so $\alpha_k^2 + \beta_k^2 = 1$.

The current estimate of λ_1 is $\widehat{\lambda}_k = \rho_A(u_k) = (u_k^T A u_k)/(u_k^T u_k)$. Then

$$\begin{aligned} \widehat{\lambda}_k &= \lambda_1 \alpha_k^2 + 2\alpha_k \beta_k \lambda_1 u^T s_k + \beta_k^2 s_k^T A s_k = \lambda_1 \alpha_k^2 + \beta_k^2 s_k^T A s_k \\ &= \lambda_1 + \beta_k^2 (s_k^T A s_k - \lambda_1). \end{aligned} \tag{3.1}$$

The residual vector is

$$\begin{aligned} r_k = Au_k - \widehat{\lambda}_k u_k &= \beta_k (A s_k - \lambda_1 s_k) + \alpha_k \beta_k^2 (\lambda_1 - s_k^T A s_k) u + \beta_k^3 (\lambda_1 - s_k^T A s_k)\, s_k \\ &= \beta_k (A - \lambda_1 I) s_k + O(\beta_k^2). \end{aligned}$$

Therefore the vector added to the Davidson subspace is

$$t_k = M r_k = \beta_k M (A - \lambda_1 I) s_k + O(\beta_k^2).$$

The new eigenvalue and eigenvector estimates are the smallest Ritz value and its Ritz vector, respectively, for the expanded subspace. Thus the new eigenvalue estimate $\widehat{\lambda}_{k+1} \leq \rho_A(\widehat{u}_k)$ where $\widehat{u}_k$ is a linear combination of u_k and t_k. The vector $\widehat{u}_k$ will be chosen in such a way that the convergence rate of the method is more easily demonstrated.

To compute $\rho_A(\widehat{u}_k)$ to an accuracy of $O(\beta_k^3)$, we use the following approximation to $\rho_A(u + \delta u)$ where $\delta u = O(\beta_k) \ll 1$:

$$
\begin{aligned}
\rho_A(u+\delta u) &= (u+\delta u)^T A(u+\delta u)/(u+\delta u)^T(u+\delta u) \\
&= (u^TAu + 2u^TA\delta u + \delta u^TA\delta u)/(u^Tu + 2u^T\delta u + \delta u^T\delta u) \\
&= (\lambda_1 + 2\lambda_1 u^T\delta u + \delta u^TA\delta u)/(1 + 2u^T\delta u + \delta u^T\delta u) \\
&= (\lambda_1 + 2\lambda_1 u^T\delta u + \delta u^TA\delta u) \\
&\qquad \times(1 - 2u^T\delta u - \delta u^T\delta u + 4(u^T\delta u)^2 + O(\|\delta u\|^3)) \\
&= \lambda_1 - \lambda_1\delta u^T\delta u + \delta u^TA\delta u + O(\|\delta u\|^3) \\
&= \lambda_1 + \delta u^T(A - \lambda_1 I)\delta u + O(\|\delta u\|^3).
\end{aligned} \tag{3.2}
$$

Since $\widehat{u}_k$ is a linear combination of u_k and t_k, we can choose

$$\widehat{u}_k = u_k - \gamma t_k.$$

Clearly, this is in the new Davidson subspace. Then, using (3.2), we have

$$\widehat{u}_k = \alpha_k u + \beta_k s_k - \gamma\beta_k M(A-\lambda_1 I)s_k + O(\beta_k^2) = u + \beta_k(I - \gamma M(A-\lambda_1 I))s_k + O(\beta_k^2).$$

Thus with $\delta u = \beta_k(I - \gamma M(A-\lambda_1 I))s_k + O(\beta_k^2)$ we obtain

$$\rho_A(\widehat{u}_k) = \lambda_1 + \beta_k^2 s_k^T(I - \gamma M(A-\lambda_1 I))^T(A-\lambda_1 I)(I - \gamma M(A-\lambda_1 I))s_k + O(\beta_k^3).$$

Now, P is the orthogonal projection onto $\ker(A-\lambda_1 I)^\perp$. Since $\ker(A-\lambda_1 I)^\perp =$ range P, it follows that $(A-\lambda_1 I) = (A-\lambda_1 I)P$, and using transposes and symmetry, we have $(A-\lambda_1 I) = P(A-\lambda_1 I)$. Since $(A-\lambda_1 I)$ is a symmetric positive semi-definite matrix, it has a symmetric positive semi-definite square root [10, p. 405], which is denoted $(A-\lambda_1 I)^{1/2}$. Then $\rho_A(\widehat{u}_k)$ can be written as

$$
\begin{aligned}
&\lambda_1 + \beta_k^2 s_k^T(I - \gamma MP(A-\lambda_1 I))^T P(A-\lambda_1 I)P(I - \gamma MP(A-\lambda_1 I))s_k + O(\beta_k^3) \\
&= \lambda_1 + \beta_k^2 s_k^T(P - \gamma PMP(A-\lambda_1 I))^T(A-\lambda_1 I)(P - \gamma PMP(A-\lambda_1 I))s_k + O(\beta_k^3) \\
&= \lambda_1 + \beta_k^2 s_k^T(P - \gamma PMP(A-\lambda_1 I))^T(A-\lambda_1 I)^{1/2} \\
&\qquad \times(A-\lambda_1 I)^{1/2}(P - \gamma PMP(A-\lambda_1 I))s_k + O(\beta_k^3) \\
&= \lambda_1 + \beta_k^2\|(A-\lambda_1 I)^{1/2}(P - \gamma PMP(A-\lambda_1 I))s_k\|_2^2 + O(\beta_k^3).
\end{aligned} \tag{3.3}
$$

But

$$(A-\lambda_1 I)^{1/2}(P - \gamma PMP(A-\lambda_1 I)) = (P - \gamma(A-\lambda_1 I)^{1/2}PMP(A-\lambda_1 I)^{1/2})(A-\lambda_1 I)^{1/2}$$

since $(A-\lambda_1 I)^{1/2}P = P(A-\lambda_1 I)^{1/2} = (A-\lambda_1 I)^{1/2}$. Applying this to the expression for $\rho_A(\widehat{u}_k)$ in equation (3.3), we have

$$
\begin{aligned}
\rho_A(\widehat{u}_k) &= \lambda_1 + \beta_k^2\|(P - \gamma(A-\lambda_1 I)^{1/2}PMP(A-\lambda_1 I)^{1/2})(A-\lambda_1 I)^{1/2}s_k\|_2^2 + O(\beta_k^3) \\
&\leq \lambda_1 + \beta_k^2\|P - \gamma(A-\lambda_1 I)^{1/2}PMP(A-\lambda_1 I)^{1/2}\|_2^2\,\|(A-\lambda_1 I)^{1/2}s_k\|_2^2 + O(\beta_k^3)
\end{aligned}
$$

Furthermore from the definition $\sigma = \|P - \gamma(A-\lambda_1 I)^{1/2}PMP(A-\lambda_1 I)^{1/2}\|_2$, we can write

$$
\begin{aligned}
\rho_A(\widehat{u}_k) &\leq \lambda_1 + \beta_k^2\sigma^2\|(A-\lambda_1 I)^{1/2}s_k\|_2^2 + O(\beta_k^3) \\
&= \lambda_1 + \beta_k^2\sigma^2 s_k^T(A-\lambda_1 I)s_k + O(\beta_k^3).
\end{aligned} \tag{3.4}
$$

Since $\widehat{\lambda}_{k+1} \leq \rho_A(\widehat{u}_k)$, and $\widehat{\lambda}_k = \lambda_1 + \beta_k^2 s_k^T(A - \lambda_1 I)s_k$,

$$0 \leq \widehat{\lambda}_{k+1} - \lambda_1 \leq \sigma^2(\widehat{\lambda}_k - \lambda_1) + O(\beta_k^3). \tag{3.5}$$

Consequently the convergence of the eigenvalue estimates is geometric with convergence factor σ^2:

$$\frac{\widehat{\lambda}_{k+1} - \lambda_1}{\widehat{\lambda}_k - \lambda_1} \leq \sigma^2 + O(\beta_k). \tag{3.6}$$

If $\lambda_2 > \lambda_1$ is the second *distinct* eigenvalue, then using (3.1) we have

$$\rho_A(u_k) \geq \lambda_1 + (\lambda_2 - \lambda_1)\beta_k^2,$$

and so

$$\beta_k^2 \leq \frac{\widehat{\lambda}_k - \lambda_1}{\lambda_2 - \lambda_1}.$$

Thus

$$|\beta_{k+1}| \leq \sqrt{\frac{\widehat{\lambda}_{k+1} - \lambda_1}{\lambda_2 - \lambda_1}} \leq (\sigma + O(\beta_k))\sqrt{\frac{\widehat{\lambda}_k - \lambda_1}{\lambda_2 - \lambda_1}}$$

which shows that $\beta_k \to 0$ geometrically with convergence factor σ.

As $\beta_k = \sin \angle(u_k, u)$, it follows that the angle between the exact and computed eigenvectors converges geometrically as desired. □

4. Further bounds. The main difficulty of the above results is that it is extremely difficulty to test the hypotheses for any particular matrix. What would be most significant are conditions for the convergence bound which are known to be satisfied by particular existing linear system preconditioners. For example, consider multigrid preconditioners M for matrices A arising from elliptic partial differential equations discretizations; it can be shown that $\|MA\|_2$ and $\|(MA)^{-1}\|_2$ are both bounded independently of the size of the matrix A [3, 19].

We now seek similar conditions which will at least give convergence rates independent of the size of the problem under consideration. As an illustration of the grid-independence of the convergence rate that is observed in practice, see Figure 4.1. This figure shows results for the Generalized Davidson algorithm modified for calculating several eigenvalues. This eigensolver for several eigenvalues was first presented in [12]. In this variant, the Generalized Davidson algorithm finds the eigenvalues in order. Initially the first or smallest eigenvalue of S_k is used; once that eigenvalue gives a good estimate of the first eigenvalue of A, the next eigenvalue of S_k is used for estimating the next eigenvalue of A, and so on. The graph in Figure 4.1 shows the residual norms $||Ax_k - \widehat{\lambda}_k x_k||$ of the iterates of the the GD algorithm applied to the Laplacian on a square, for various grid sizes. The preconditioner used is an implementation of a (2,1)-FMV method (Full Multigrid V-cycle) [11] with a red-black Gauss–Seidel smoother, which is independent of the current eigenvalue sought. The grid-independence of the convergence rates is observed during the convergence of each one of the eigenvalues sought. More numerical results are shown in [12] and a new parallel version of the GD algorithm was presented in [2].

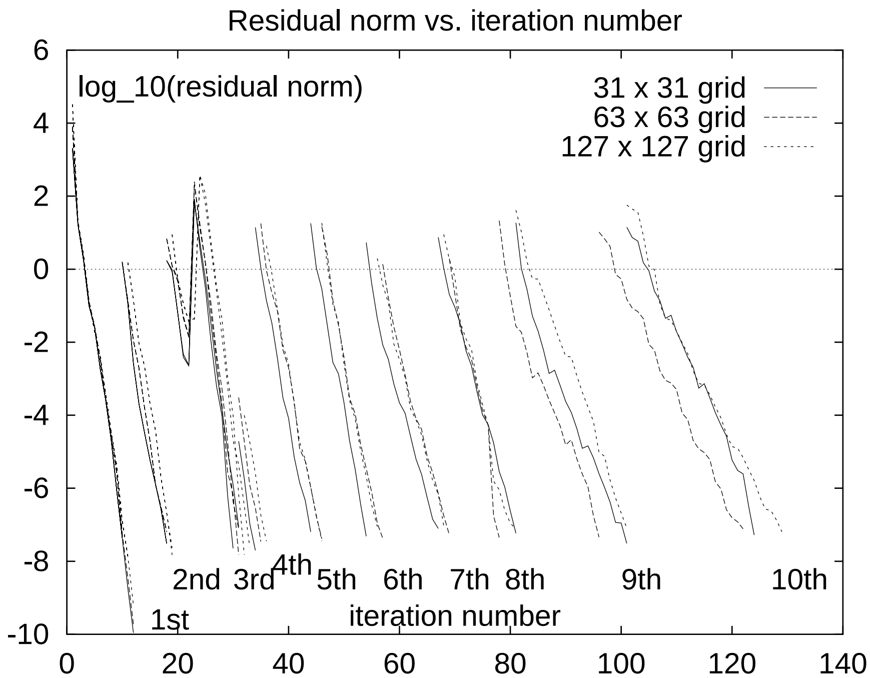

FIG. 4.1. *Residual norm ($\|Au_k - \widehat{\lambda}_k u_k\|_2/\|u_k\|_2$) vs. iteration number (k)*

GD algorithms for finding one eigenvalue, seek the first (i.e., smallest) eigenvalue λ_1 of A, and the preconditioner for GD can be a fixed matrix or operator, M. Let P denote the orthogonal projection onto the space perpendicular to Null $(A - \lambda_1 I)$. Since P and $I - P$ are projections onto eigenspaces of A, $AP = PA$, and in fact, P commutes with every power of A. In the following we use the notation $\rho(B)$ to denote the spectral radius of B.

THEOREM 4.1. *Suppose that:*

1. *A and M are symmetric, positive definite.*
2. *$\|MA\|_2$, $\|(MA)^{-1}\|_2 \leq c_1$*

for some positive constant c_1. Then the asymptotic convergence factor of the eigenvectors u_k produced by Algorithm 1 is bounded above by a constant which depends only on c_1 and $\lambda_1 < \lambda_2$ (the first two distinct eigenvalues). In particular, we can bound the asymptotic convergence factor by $(1 - (1 - \lambda_1/\lambda_2)/c_1^2)/(1 + (1 - \lambda_1/\lambda_2)/c_1^2)$.

Proof. Note that the asymptotic convergence factor in Theorem 3.1 is bounded above by $\sigma = \|P - \gamma P(A - \lambda_1 I)^{1/2} PMP(A - \lambda_1 I)^{1/2} P\|_2$. In this proof we will bound σ in terms of the relative spectral gap and $\kappa_2(MA)$. To do this we need to find upper and lower bounds on the matrix inside the norm. The main tools are matrix inequalities ($A \leq B$ means that $u^T Au \leq u^T Bu$ for all u), the fact that AB and BA have the same spectra, and positive definite square roots of positive definite matrices.

Note that $(A - \lambda_1 I)^{1/2} M (A - \lambda_1 I)^{1/2}$ is similar to

$$M^{1/2}(A - \lambda_1 I)M^{1/2} \leq M^{1/2} A M^{1/2}.$$

$M^{1/2}AM^{1/2}$ is similar to MA, and so $\rho(M^{1/2}AM^{1/2}) = \rho(MA) \leq \|MA\|_2$. Thus, $\|(A - \lambda_1 I)^{1/2} M (A - \lambda_1 I)^{1/2}\|_2 = \rho((A - \lambda_1 I)^{1/2} M (A - \lambda_1 I)^{1/2}) \leq \|MA\|_2 \leq c_1$. Hence, $(A - \lambda_1 I)^{1/2} M (A - \lambda_1 I)^{1/2} \leq c_1 I$, and consequently, $P(A - \lambda_1 I)^{1/2} M(A -$

$\lambda_1 I)^{1/2}P \le c_1 P$ and

$$P - \gamma P(A - \lambda_1 I)^{1/2} PMP(A - \lambda_1 I)^{1/2} P \ge (1 - \gamma c_1)P.$$

To obtain an inequality in the reverse direction, consider $u \in \text{Range}\, P$ in the expression $w = u^T(P - \gamma P(A - \lambda_1 I)^{1/2} M(A - \lambda_1 I)^{1/2} P)u$. Since $P - \gamma P(A - \lambda_1 I)^{1/2} M(A - \lambda_1 I)^{1/2} P = P(I - \gamma(A - \lambda_1 I)^{1/2} M(A - \lambda_1 I)^{1/2})P$ and $Pu = u$, $w = u^T(I - \gamma(A - \lambda_1 I)^{1/2} M(A - \lambda_1 I)^{1/2})u$. Now,

$$\begin{aligned} u^T u - w &= \gamma u^T (A - \lambda_1 I)^{1/2} M (A - \lambda_1 I)^{1/2} u \\ &= \gamma u^T (I - \lambda_1 A^{-1})^{1/2} A^{1/2} M A^{1/2} (I - \lambda_1 A^{-1})^{1/2} u \\ &\ge \gamma \lambda_{min}(A^{1/2} M A^{1/2}) \|(I - \lambda_1 A^{-1})^{1/2} u\|_2^2. \end{aligned}$$

But, since $u \in \text{Range}\, P = (\text{Null}\,(A - \lambda_1 I))^{\perp}$,

$$\|(I - \lambda_1 A^{-1})^{1/2} u\|_2^2 = u^T (I - \lambda_1 A^{-1}) u = \|u\|_2^2 - \lambda_1 u^T A^{-1} u \ge (1 - \lambda_1/\lambda_2)\|u\|_2^2.$$

Also, we can give a lower bound on $\lambda_{min}(A^{1/2} M A^{1/2})$ as follows. Since $A^{1/2} M A^{1/2}$ is symmetric positive definite, $\lambda_{min}(A^{1/2} M A^{1/2}) = 1/\rho((A^{1/2} M A^{1/2})^{-1})$ $= 1/\rho(A^{-1/2} M^{-1} A^{-1/2})$. This latter matrix is similar to $A^{-1} M^{-1} = (MA)^{-1}$, so $\lambda_{min}(A^{1/2} M A^{1/2}) \ge 1/\|(MA)^{-1}\|_2 \ge 1/c_1$.

Thus,

$$u^T (A - \lambda_1 I)^{1/2} M (A - \lambda_1 I)^{1/2} u \ge (1 - \lambda_1/\lambda_2)\|u\|_2^2 / c_1,$$

and so

$$w \le \|u\|_2^2 - \gamma(1 - \lambda_1/\lambda_2)\|u\|_2^2/c_1 = (1 - \gamma(1 - \lambda_1/\lambda_2)/c_1)\|u\|_2^2.$$

In terms of matrix inequalities,

$$(1 - \gamma c_1)P \le P - \gamma P(A - \lambda_1 I)^{1/2} PMP(A - \lambda_1 I)^{1/2} P \le (1 - \gamma(1 - \lambda_1/\lambda_2)/c_1)P.$$

Combining these two inequalities we see that

$$\|P - \gamma P(A - \lambda_1 I)^{1/2} PMP(A - \lambda_1 I)^{1/2} P\|_2 \le \max(|1 - \gamma c_1|, |1 - \gamma(1 - \lambda_1/\lambda_2)/c_1|).$$

By choosing $\gamma = 2/(c_1 + (1 - \lambda_1/\lambda_2)/c_1)$, we minimize this bound, giving

$$\|P - \gamma P(A - \lambda_1 I)^{1/2} PMP(A - \lambda_1 I)^{1/2} P\|_2 \le \frac{1 - (1 - \lambda_1/\lambda_2)/c_1^2}{1 + (1 - \lambda_1/\lambda_2)/c_1^2}.$$

Thus the asymptotic convergence factor is bounded above by

$$\frac{1 - (1 - \lambda_1/\lambda_2)/c_1^2}{1 + (1 - \lambda_1/\lambda_2)/c_1^2},$$

which is the desired bound on σ. □

The above bound for the convergence factor (cf) can be used to derive the formula $(1 - cf)/(1 + cf) \ge (1 - \lambda_1/\lambda_2)/c_1^2$. Figure 4.2 confirms that in fact this is the case with the multigrid preconditioned GD applied to our test problem. The vertical axis is data obtained from the numerical results in Figure 4.1, the horizontal axis is the right side of this later inequality (assuming $c_1 = 1$). As predicted, the values on the left side of the inequality are always above the identity line.

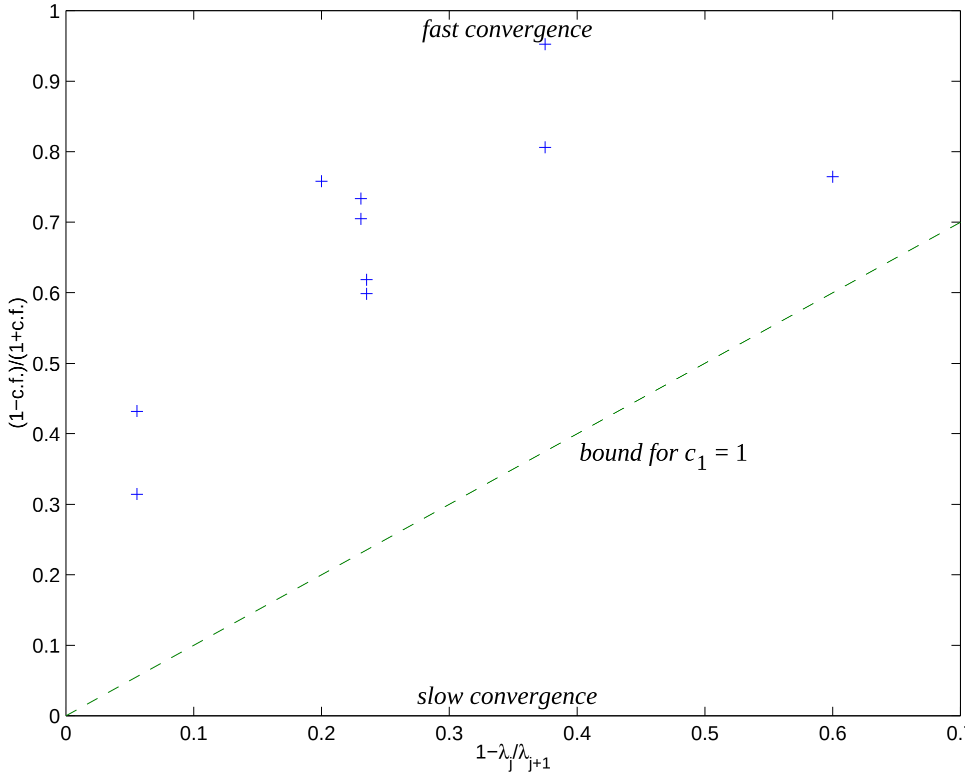

FIG. 4.2. *Numerical convergence results estimates compared with* $1 - \lambda_j/\lambda_{j+1}$

5. Conclusions. In the preconditioning step of the Generalized Davidson Algorithm, given the condition number $\kappa_2(MA)$, we can scale M so that $\|MA\|_2$, $\|(MA)^{-1}\|_2 \le \sqrt{\kappa_2(MA)}$. Since scaling does not affect the iterates of the algorithm, the convergence rate is unchanged. This gives a bound on the convergence factor of $(1-(1-\lambda_1/\lambda_2)/\kappa_2(MA))/(1+(1-\lambda_1/\lambda_2)/\kappa_2(MA))$. Thus the bound derived here implies that the number of iterations needed to achieve a residual norm $\|Au_k - \widehat{\lambda}_k u_k\|_2/\|u_k\|_2 < \epsilon$ to be, asymptotically, $O(\log(1/\epsilon)\kappa_2(MA)/(1-\lambda_1/\lambda_2))$. That is, the number of iterations is proportional to the condition number of the preconditioned matrix MA, and inversely proportional to the relative spectral gap $1-\lambda_1/\lambda_2$. This bound is independent of the size of the problem as the results of Figure 4.1 suggest.

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