DAVIDSON DIAGONALIZATION METHOD AND ITS APPLICATION TO ELECTRONIC STRUCTURE CALCULATION*

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Abstract.

Davidson algorithm is a subspace iterative diagonalization method, which appends to the subspace with modified (preconditioned) residue vectors during the iteration process, in contrast to Krylov space methods. In this report, different views of understanding Davidson-type methods are reviewed, and a variety of ways of generating the new expansion vector are implemented in Matlab and their performances compared. It is observed that the original Davidson method converges fast for diagonally dominant matrices, but relatively slow otherwise, which could be fixed to some extent by using modified methods. A "quasi-realistic" problem, the diagonalization of the Hamiltonian of a planewave-pseudopotential based electronic structure calculation, is solved using Davidson methods, and the result is compared with the other mainstream algorithm, preconditioned non-linear Conjugate Gradient (CG) method.

Key words. Iterative Diagonalization, Subspace Methods, Davidson Method

1. Introduction. Large-scale symmetric eigenvalue problems arise from a variety of contexts of scientific and engineering computing, and examples include configuration interaction calculations in quantum chemistry, electronic structure calculation of solids, and solving eigenmodes of electromagnetic wave propagation, etc. In some application, only the lowest one or few eigenpairs are of interest. If the dimension of the problem is not "too large", *direct* or *dense* methods are available[1], the cost of which grows like N^3 and the direct access memory requirements grows liks N^2. When N becomes much larger, however, the direct methods are not affordable any more, and iterative methods are generally used in search of the lowest (or highest, or some specific ones) eigenpairs. One of the most important categories of iterative eigen algorithms consists of subspace methods[2], whose general principle is to project the full matrix into smaller subspace, solve a smaller eigen problem in the subspace, and use the eigenvalues and eigenvectors in the subspace problem (they are called *Ritz values* and *Ritz vectors*) to approximate the true eigenpairs. Krylov space algorithms (such as Lanczos algorithm) are familiar examples of subspace methods, which construct the subspace given matrix $\mathbf{H}$ and initial guess vector $\mathbf{b}$ as the span of vectors $\{\mathbf{b}, \mathbf{Hb}, \mathbf{H}^2\mathbf{b}, ..., \mathbf{H}^{n-1}\mathbf{b})\}$. Although the Krylov space methods elegantly demonstrate how to construct and expand the subspace, they usually fail to favor certain eigenpair that is wanted, and lead to slow convergence.

Davidson[3] came up with an idea of expanding the subspace in such a way that certain eigenpair(s) would be favored. Bearing in mind the fact that if certain true eivenvector lies in the subspace of current iteration, the eigen problem in the subspace would give the exact corresponding eigenpair. Thus to achieve fast convergence, a better way to expand the subspace is to choose the new expansion vector to be the component of the error vector which is orthogonal to the subspace[2]. If this orthogonal component could be solved exactly and added to the subspace, then convergence

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is guaranteed to be achieved in the next iteration (in exact arithmetic).

Denote the true eigenvector as $\mathbf{v}$, the current approximate eigenvector as $\mathbf{x}$, the orthogonal component of the error vector as δ, and the eigen equation becomes

$$\mathbf{H}(\mathbf{x}+\delta) = \lambda(\mathbf{x}+\delta), \tag{1.1}$$

In above λ is the true eigenvalue, and can be writen as $\lambda = \rho + \epsilon$, with $\rho = \mathbf{x}^T\mathbf{H}\mathbf{x}$ being the *Rayleigh quotient* and ϵ being the error. And equation (1.1) can be rewritten as

$$\begin{aligned}(\mathbf{H}-\rho-\epsilon)\delta &= -(\mathbf{H}-\rho-\epsilon)\mathbf{x} \\ &= -\mathbf{r}+\epsilon\mathbf{x}\end{aligned} \tag{1.2}$$

Here $\mathbf{r} = (\mathbf{H}-\rho\mathbf{I})\mathbf{x}$ is the residue vector at current iteration step. Solving δ and appending it to the subspace is the essence of Davidson methods, but since solving δ from equation (1.2) is nontrivial (a linear system with the same dimension as the original problem), different schemes of obtaining δ in an approximate but efficient way are devised, forming various flavors of Davidson methods, which will be reviewed in the following subsections. Here, the main steps in a typical Davidson algorithm are sketched below:

Initialization To solve the lowest k eigenvectors, a guess eigenspace with dimension l ($l \geq k$) and orthonormal basis $\{\mathbf{b}_1, \mathbf{b}_2, ..., \mathbf{b}_l\}$ is constructed

Subspace Problem Form the matrix-vector products $\{\mathbf{H}\mathbf{b}_1, \mathbf{H}\mathbf{b}_2, ..., \mathbf{H}\mathbf{b}_l\}$, and calculate the matrix elements in the subspace $\widetilde{\mathbf{H}}_{ij} = \mathbf{b}_i^T\mathbf{H}\mathbf{b}_j$, and solve for the eigenvalues $\{\rho_i\}$ and eigenvectors $\{\mathbf{x}_i\}$ in the subspace as the approximate eigenpairs.

Compute Residue Calculate the residue vector $\mathbf{r}_i = (\mathbf{H}-\rho_i\mathbf{I})\mathbf{x}_i$, and check if the convergence is achieved as $\|\mathbf{r}_i\| \leq$ tolerance. If the convergence is not achieved, continue to the next step.

Compute Correction Vector Calculate the correction vector based on the residue vector and approximate eigenpairs. This part is where the main variations of the algorithm exist, and has large impact on the performance. Different schemes will be discussed in detail in later sections.

Expand the Subspace Orthogonalize the correction vector to the previous subspace using (modified) Gram-Schmidt scheme, and append the orthonormalized correction vector to the previous subspace and repeat the iteration from step 2 (only matrix elements involved with the new vector need to be computed) until the convergence is achieved.

1.1. Diagonal-Preconditioned-Residue (DPR) method. In his original paper, Davidson[3] argued that for diagonally dominant matrices, one can replace $\mathbf{H}$ in (1.2) by its diagonals (denoted as $\mathbf{D}$ here), and assume ϵ is negligible, thus can be removed from (1.2), and one ends up with the equation

$$\delta = -(\mathbf{D}-\rho\mathbf{I})^{-1}\mathbf{r} \tag{1.3}$$

Although the equation (1.3) now becomes trivial to solve, the approximations made seem too crude at the first sight. It turns out that there are different ways of understanding this correction vector δ, which give more motivations and insights. Consider the Rayleigh quotient of the trial eigenvector $\mathbf{x}$

$$\rho(\mathbf{x}) = \frac{\mathbf{x}^T\mathbf{H}\mathbf{x}}{\mathbf{x}^T\mathbf{x}} \tag{1.4}$$

Now we would like to minimize the Rayleigh quotient by varying $\mathbf{x}$, but instead of varying $\mathbf{x}$ along certain direction (as we usually do in steepest descent and conjugate gradient method), we vary one component of $\mathbf{x}$ while holding all the other components fixed. Specifically, if one varies the ith component x_i by an amount δ_i, the optimum choice of δ_i from

$$\left.\frac{\partial \rho}{\partial x_i}\right|_{x_i+\delta_i} = 0 \tag{1.5}$$

is just given by

$$\delta_i = -(\mathbf{H}_{ii} - \rho)^{-1} r_i \tag{1.6}$$

This expression looks similar to (1.3), except that ρ and r_i here are evaluated at $\mathbf{x} + \delta_i \mathbf{e}_i$. In this sense the correction vector given by equation (1.3) could also be interpreted as an approximation of the optimum variation vector that minimizes the Rayleigh quotient locally. A third interpretation of equation (1.3) has to do with *Rayleigh Quotient Inverse Iteration* (RQII)[4]. Consider a RQII step

$$\mathbf{x}^{new} = (\mathbf{H} - \rho)^{-1}\mathbf{x} \tag{1.7}$$

It was shown in class that RQII exhibits cubic convergence when the approximate eigenvector approaches the true one. Now if one imposes that the correction in each step be orthogonal to the previous trial vector, i.e. $\mathbf{x}^{new} = (\mathbf{x} + \delta)/\epsilon$, where $\mathbf{x}^T\delta = 0$ and ϵ plays a role as the normalization factor, then equation (1.7) could be rewritten as (according to Davidson[3], a modified Newton-Raphson equation)

$$\mathbf{x} + \delta = (\mathbf{H} - \rho\mathbf{I})^{-1}\mathbf{x}/\epsilon \tag{1.8}$$

After operating $\mathbf{x}^T(\mathbf{H} - \rho\mathbf{I})^{-1}$ on both sides on the left, ϵ can be solved as

$$\epsilon = \frac{1}{\mathbf{x}^T(\mathbf{H} - \rho\mathbf{I})^{-1}\mathbf{x}} \approx \lambda - \rho \tag{1.9}$$

This observation is consistent with the previous discussions. Given ϵ the equation (1.8) can be rewritten as

$$(\rho\mathbf{I} - \mathbf{H})(\mathbf{x} + \delta) \approx \epsilon\mathbf{x} \tag{1.10}$$

$$(\rho - \mathbf{H}_{ii})\delta_i \approx r_i + \sum_{j\neq i} \mathbf{H}_{ij}\delta_j + \epsilon\mathbf{x}_i \tag{1.11}$$

From this point of view, equation (1.3) is also an approximate form of an orthogonal correction vector in one step of RQII. Davidson[5] and Pulay[6] also pointed out that equation (1.3) is a form of diagonal-preconditioned (Jacobi-type) gradient of the Rayleigh quotient, after which this original Davidson method is also referred to as Diagonal-Preconditioned-Residue (DPR) method. From the discussion given above, especially the approximation made along the way, one can tentatively predict that this original flavor only works well in diagonally dominant matrices, which will be verified in experiments shown in the next two sections.

1.2. Improved versions: IIGD, GJD and RQII. Some slightly modified versions of Davidson methods were proposed in late 80s and 90s, and the basic idea was to add correction terms that were dropped in the original version back and try to maintain an efficient way of evaluating the correction vector. A brief review was given in the Appendix of reference[11]. Olsen *et al.*[4] proposed that adding the $\epsilon\mathbf{x}$ term back and the correction vector can be given by

$$\delta = (\mathbf{D} - \rho\mathbf{I})^{-1}(-\mathbf{r} + \epsilon\mathbf{x}) \tag{1.12}$$

By enforcing the orthogonality relation $\mathbf{x}^T\delta = 0$, ϵ can be solved as

$$\epsilon = \frac{\mathbf{x}^T(\mathbf{D} - \rho\mathbf{I})^{-1}\mathbf{r}}{\mathbf{x}^T(\mathbf{D} - \rho\mathbf{I})^{-1}\mathbf{x}} \tag{1.13}$$

Because of the resemblance of the correction vector to that from RQII, this method was named as *Invers-Iteration generalized Davidson (IIGD)* method.

Sleijpen *et al.*[7][8][9] suggested a further improvement over IIGD, the *Generalized Jacobi Davidson (GJD)*, which is also explained in detail in the online book *Templates for the Solution of Algebraic Eigenvalue Problems*[2]. By operating on both sides of the RQII equation (1.10) the projector $(1 - \mathbf{x}\mathbf{x}^T)$, ϵ can be removed explicitly from the equation, and after reorganizing the RQII equation can be written as a projected form

$$(\mathbf{I} - \mathbf{x}\mathbf{x}^T)(\mathbf{H} - \rho\mathbf{I})(\mathbf{I} - \mathbf{x}\mathbf{x}^T)\delta = -\mathbf{r} \tag{1.14}$$

Here $\widetilde{\mathbf{H}} = (\mathbf{I} - \mathbf{x}\mathbf{x}^T)(\mathbf{H} - \rho\mathbf{I})(\mathbf{I} - \mathbf{x}\mathbf{x}^T)$ is the projected matrix onto the subspace which is orthogonal to $\mathbf{x}$. In the original paper it is suggested to solve the equation (1.14) approximately, for example, by some steps of MINRES. But in practice, any efficient iterative linear solver (conjugate gradient, for example) can be utilized to solve the GJD equation at each iteration step. Along the same path, it is also possible to solve the RQII equation directly at each step by efficient linear solvers. By including more correction terms back into the original recipe, these improved versions aim at improving the performance of Davidson method when applied to non-diagonally-dominant matrices. The results and comparison will be given in subsequent sections.

There are other modifications to Davidson methods, which are mainly concerned about optimizing the correction vector and speeding up the convergence. Since space is limited, those minor modifications will not be described here, and a thorough review by Leininger *et al.*[10] is available.

1.3. Subspace Projected Approximate Matrix (SPAM) modification. Taking into account the fact that when the matrix dimension becomes extremely large, the most time-consuming parts of the iterative algorithms are the matrix-vector products, an extension of Davidson method called *Subspace Projected Approximate Matrix (SPAM)*[11] was designed, aiming at reducing number of "exact" matrix-vector products as much as possible, in a flexible and adaptive way. Assume at certain iteration step, the subspace vectors are given by columns of matrix $\mathbf{B}$, and the matrix-vector products are computed as columns of matrix $\mathbf{W}$.Thus the subspace representation of $\mathbf{H}$ is given by $\bar{\mathbf{H}} = \mathbf{B}^T\mathbf{H}\mathbf{B} = \mathbf{B}^T\mathbf{W}$. Define the orthogonal projector $\mathbf{P} = \mathbf{B}^T\mathbf{B}$ and the complementary projector $\mathbf{Q} = \mathbf{I} - \mathbf{P}$, then the original matrix $\mathbf{H}$ can be written equivalently as

$$\mathbf{H} = (\mathbf{P} + \mathbf{Q})\mathbf{H}(\mathbf{P} + \mathbf{Q})$$

$$
\begin{aligned}
&= \mathbf{PHP} + \mathbf{PHQ} + \mathbf{QHP} + \mathbf{QHQ} \\
&= (\mathbf{B}\bar{\mathbf{H}}\mathbf{B}^T + \mathbf{B}\mathbf{W}^T\mathbf{Q} + \mathbf{Q}\mathbf{W}\mathbf{X}^T) + \mathbf{QHQ}
\end{aligned} \tag{1.15}
$$

When computing the matrix-vector product $\mathbf{Hy}$, the first three terms in equation (1.15) are easy to handle since $\mathbf{B}$ and $\mathbf{W}$ are available and have low dimensions. The basic idea of SPAM algorithm is to approximate $\mathbf{H}$ in the fourth term by another matrix $\mathbf{H^1}$ whose matrix-vector products $\mathbf{H^1y}$ require less effort to compute. Choice of $\mathbf{H^1}$ is flexible and problem-dependent and can be a less dense matrix than $\mathbf{H}$ or some formal or algebraic approximation to $\mathbf{H}$. Given $\mathbf{H^1}$, the original matrix $\mathbf{H}$ can now be approximated by a "SPAM" matrix $\mathbf{H}^{SPAM}$

$$
\mathbf{H}^{SPAM} = (\mathbf{B}\bar{\mathbf{H}}\mathbf{B}^T + \mathbf{B}\mathbf{W}^T\mathbf{Q} + \mathbf{Q}\mathbf{W}\mathbf{X}^T) + \mathbf{Q}\mathbf{H^1}\mathbf{Q} \tag{1.16}
$$

One good property of $\mathbf{H}^{SPAM}$ is that for any vector $\mathbf{y} \in span(\mathbf{B})$, equation (1.16) indicates that $\mathbf{H}^{SPAM}\mathbf{y} = \mathbf{Hy}$, which means if the column space of $\mathbf{B}$ converges to the eigenspace of $\mathbf{H}^{SPAM}$, this eigenspace is exactly the eigenspace of $\mathbf{H}$. Thus one can solve the eigenproblem of $\mathbf{H}^{SPAM}$ instead and use the eigenvectors of $\mathbf{H}^{SPAM}$ to append to the previous subspace ($span(\mathbf{B})$). To update $\mathbf{W}$, one "exact" matrix-vector product involving $\mathbf{H}$ is required. To solve the eigenproblem of $\mathbf{H}^{SPAM}$ (with the same dimension as the original problem), an iterative Davidson method is utilized, which would be cheap, thanks to another good property of $\mathbf{H}^{SPAM}$: for any vector $\mathbf{x}_\perp$ orthogonal to the column space of $\mathbf{B}$, the matrix-vector product takes the simple form

$$
\mathbf{H}^{SPAM}\mathbf{x}_\perp = \mathbf{w}^1 + \mathbf{B}(\mathbf{W}^T\mathbf{x}_\perp - \mathbf{B}^T\mathbf{w}^1) \tag{1.17}
$$

where $\mathbf{w}^1 = \mathbf{H^1}\mathbf{x}_\perp$ is the inexpensive matrix-vector product. Here the Davidson method serves as the inner loop of an outer iterative algorithm. By virtue of this nested structure, matrix-vector products in the inner loop Davidson are cheap, whereas the outer loop "exact" matrix-vector might be expensive, but the necessary number of them are minimized. In large-scale applications, this nested structure even provides the possibility to subdivide the inner loop problem to single steps, each of which could be treated by a Davidson iteration, forming a multilevel algorithm, with more degrees of freedom to tune to adapt to specific problems.

1.4. Relation to Lanczos and Gradient-based methods. There is a close relation between Davidson method and Lanczos method[12][11]. If the diagonal-precondition part is ignored in evaluating the correction vector, i.e.

$$
\delta = -\mathbf{r} \tag{1.18}
$$

It is easily seen that the residue vector lies in an expanding Krylov space, so is the correction vector. By generating correction vectors this way Davidson method is reduced to an explicit-orthogonalization Lanczos method. Although Lanczos method seems more elegant (only two latest trial vectors need to be stored, and the subspace-projected matrix is tridiagonal), it suffers from slow convergence due to the fact that it does not selectively converge to the desired eigenpair of interest.

On the other hand, since the correction vector for the Davidson method can be interpreted as just the gradient of the Rayleigh quotient preconditioned in some

way, there are also connections between the Davidson method and gradient-based methods[1][13], such as steepest descent (SD) and conjugate gradient (CG) method. They all compute the correction vector from the residue somehow (with certain kinds of preconditioning) but use it differently: SD and CG use the correction vector as the search direction for the next step whereas Davidson methods use it to expand the subspace. Detailed comparison with respect to convergence performance in a realistic problem will be given in a later section, and also the possibility to combine these methods will be discussed.

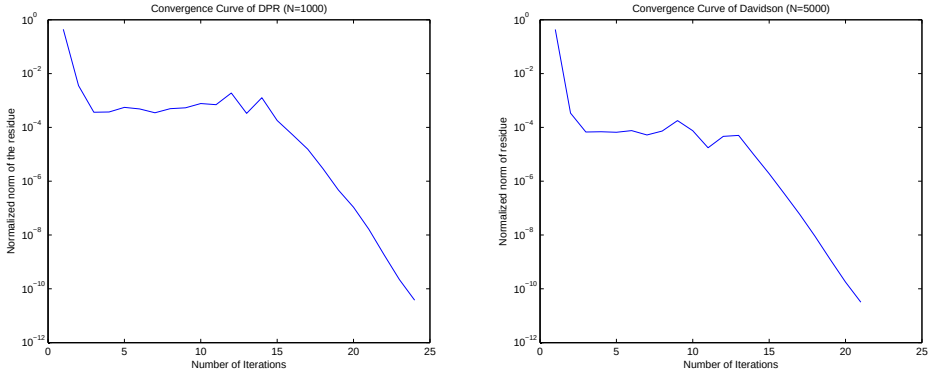
1.5. Block Davidson Method and Subspace Collapse. Another remarkable feature of Davidson method is that it can be easily extended to computing a few lowest eigenpairs simultaneously. This type of Davidson method is called *Block Davidson* or *Davidson-Liu*[14] algorithm. The basic idea is that instead of adding one new vector at each iteration, a few new vectors, corresponding to the residue vectors of different eigenpairs, will be added at each iteration, tuning the subspace eigenvetors to converge at the same time.

Another extension of Davidson method is the subspace collapse technique[6], similar to the restart scheme used in Lanczos method, which could reduce the memory requirement. The basic idea is to choose the optimal approximate eigenvectors already obtained and restart with an initial subspace expanded by the optimal approximate eigenvectors.

2. Implementation and Performance Test.

2.1. Diagonally Dominant Matrices. First the original DPR Davidson method [3][15] is implemented and applied to diagonally dominant matrices. For simplicity and convenient comparison, only the lowest eigenpair is to be solved. Block Davidson method, which solves a few lowest eigenpairs simultaneously will be demonstrated separately, but not used to compare different flavors.

The convergence performance of DPR is demonstrated in figure 2.1.



(a) $N = 1000$ (b) $N = 5000$

Fig. 2.1: The convergence curve of DPR method, applied to randomly generated diagonally dominant matrices

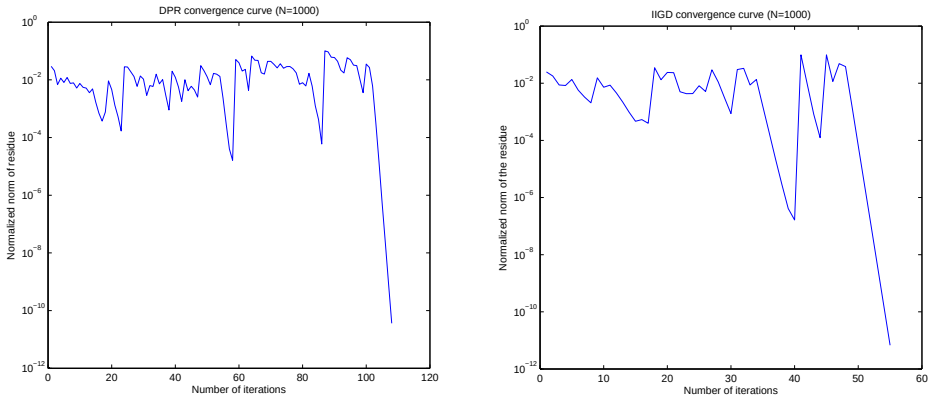
Below 30 iterations achieve the convergence of 10^{-10}, the convergence curves are

smooth and the number of iterations needed seems not to increase with the dimension of the problem, which is quite amazing. Although these convergence curves demonstrate the typical "successful" behavior of Davidson method, further study shows that the performance is much more complicated and depends on a lot of factors, and can be very sensitive. A good analysis of the convergence behavior of Davidson from the perspective of the spectrum of a preconditioned Krylov problem was given by Morgan and Scott[16]. Consider the operator $\mathbf{N}(\rho) = (\mathbf{D} - \rho\mathbf{I})^{-1}(\mathbf{H} - \rho\mathbf{I})$, then every correction vector generated during Davidson iteration is given by $\mathbf{N}$ operating on some vector. Now if ρ were a constant, then the subspace generated using Davidson iteration is just a Krylov space generated by powers of $\mathbf{N}$. Then the methods of analyzing the Krylov space methods may be considered here. Faster convergence of Arnoldi or Lanczos method can be achieved (as we learned from class) if the gap ratio (relative separation) of the spectrum of the matrix is large. Of course ρ is not a constant here, but (ideally) converges to certain eigenvalue of $\mathbf{H}$, so the spectrum of $\mathbf{N}$ when ρ is near certain eigenvalue of $\mathbf{H}$ is crucial to the convergence rate of Davidson. An extreme example is that when $\mathbf{H}$ is diagonal, then all eigenvalues of $\mathbf{N}$ are the same (1), thus Davidson method is expected to perform badly (actually fails in exact arithmetic, since $\delta = -\mathbf{x}$ in this case and lies in the previous subspace). Known from analysis of preconditioners of gradient-based methods, $(\mathbf{D} - \rho\mathbf{I})^{-1}$ tends to compress the spectrum of $(\mathbf{H} - \rho\mathbf{I})$, which is a preferred property for gradient-based methods, while in eigenvalue problems, an increased gap ratio is the desired property. From this point of view, original Davidson method is expected to perform well (or better than Lanczos method) only if after preconditioning (multiplied by $(\mathbf{D} - \rho\mathbf{I})^{-1}$) the ratio gap is increased and also the corresponding eigenvalue of $\mathbf{N}$ is not clustered with other eigenvalues. So even in the seemingly simplest case of diagonally-dominant matrices, the convergence behavior of Davidson method could be rather complicated. Figure 2.2a illustrates one typical situation where Davidson does not do so well. The algorithm seems to converge to other eigenvalues at first (corresponding to deeps in the norm of the residue) and then figures out that smaller eigenvalue exists and adjusts to it at the end. This behavior may be explained by the analysis given above that the corresponding eigenvalue of operator $\mathbf{N}$ resides in the interior instead of being well separated from other eigenvalues. IIGD is devised to improve DPR in diagonally dominant matrices, and the performance of IIGD applied to the same matrix is displayed in figure 2.2b. Although total number of iterations is reduced, stronger oscillations are observed in IIGD, which may be dangerous because if the convergence threshold is not set small enough, the algorithm may end up converging to a higher eigenvalue.

In addition to explaining when Davidson does not perform very well, the analysis given above also sheds light upon further improving Davidson method by other preconditioning method in specific problems, which will be demonstrated in a later section.

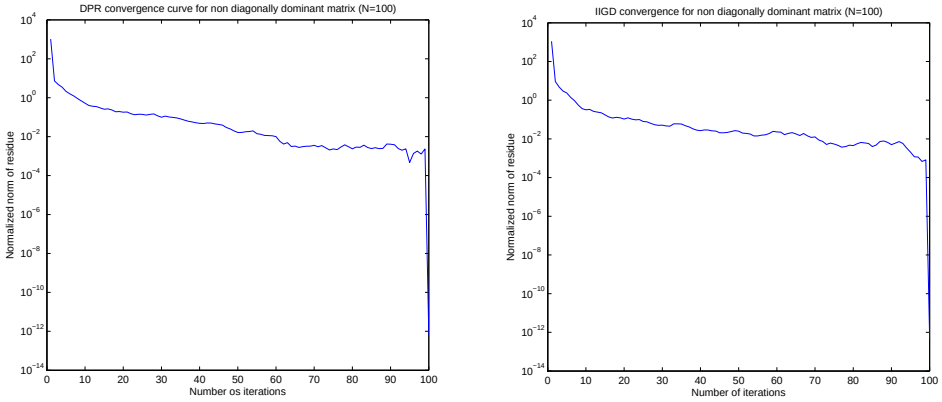
2.2. Non-Diagonally-Dominant Matrices. Figure 2.3a demonstrates how original Davidson method totally fails when dealing with non-diagonally-dominant matrices (the test matrix is generated as $\mathbf{H} = \mathbf{A}^T\mathbf{A}$, where $\mathbf{A}$ is a random matrix). Only when the dimension of the subspace is almost the same as the dimension of the original problem does the algorithm converge. This is expected since in this scenario the diagonal-preconditioning does not make improvement any more. Also shown in figure 2.3b is how IIGD also fails when applied to the same matrix.

On the other hand, GJD and RQII are devised to work in both cases (since no



(a) DPR (b) IIGD

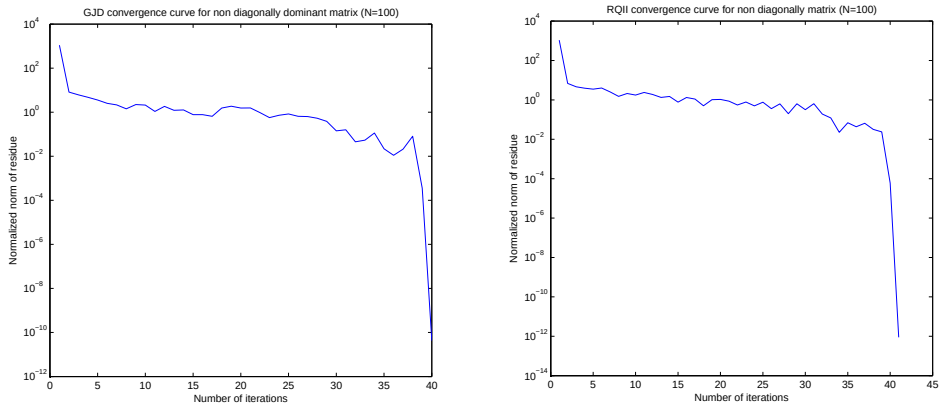
Fig. 2.2: An example of slow-converging DPR and performance of IIGD applied to the same matrix



(a) DPR (b) IIGD

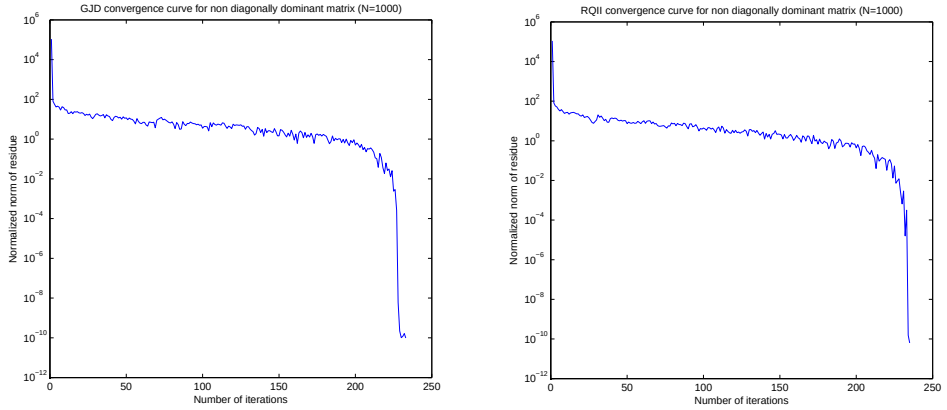
Fig. 2.3: DPR and IIGD fail in dealing with non-diagonally-dominant matrices

diagonal approximation made when solving the correction vector). Figure 2.4 demonstrates how they work when applied to the same matrix. They converge in around 40 steps, but the price to pay is (much) larger at each iteration. Another problem is that when ρ converges to certain eigenvalue, the linear system to be solved at each step is near singular, which may cause problems and slow convergence. Figure 2.5 shows that when applied to a larger non diagonally dominanat matrix, they converge slowly and other methods (such as gradient-based methods) may be more advantageous provided the increased cost at each step.



(a) GJD (b) RQII

Fig. 2.4: GJD and RQII perform better for non diagonally dominant matrices



(a) GJD (b) RQII

Fig. 2.5: GJD and RQII perform not so well for larger non diagonally dominant matrices

2.3. Block Davidson Method. To solve the lowest few eigenpairs, one can of course solve the eigenpairs one by one sequentially using Davidson from the lowest one, where at each step how to pick the correction vector is a little bit subtle[12]. A more powerful method is to solve for the lowest few eigenpairs simultaneously, using *Block Davidson Algorithm*[14]. Suppose now we are interested in the lowest k eigenpairs. Starting by a guess subspace with dimention l ($l \geq k$), the only modification to the original Davidson method is that at each step, all the correction vectors corresponding to the first k approximate eigenvectors are solved. Then orthonormalize the first correction vector against the previous subspace, and append it to the sub-

space. Repeat this process for each of the other $k-1$ correction vectors, neglecting any new vector whose norm after normalization is less than some threshold. Then solve the subspace problem again. This extension is simple and powerful, and keeps all the properties of the original Davidson method, except that the dimension of the subspace problem will grow faster during iterations.

Block Davidson Algorithm is implemented in Matlab, and the simultaneous convergence curve is show in figure 2.6.

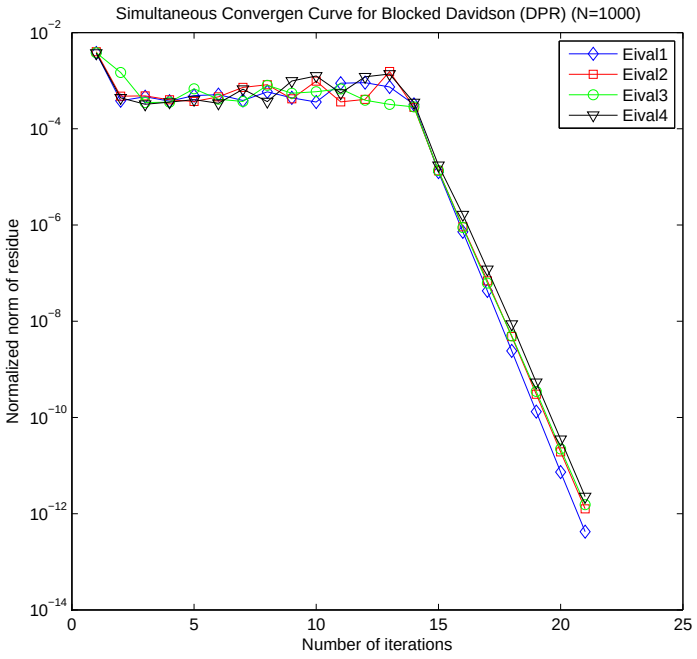


Fig. 2.6: The lowest 4 eigenvalues converge uniformly when applying Block Davidson to a 1000×1000 diagonally dominant matrix.

3. Application to a "Quasi-Realistic" Problem. First-principles calculation of electronic structures of solids has been an indispensable tool in modern research fields like material science and engineering and condensed matter physics. Among a couple of state-of-the-art methods, Pseudopotential-planewave based method[17] has long been thought of as the most natural one for the built-in periodic boundary condition. In a pseudopotential-planewave formulation, the single-electron Hamiltonian at a given point $\mathbf{k}$ in the first Brllouin zone takes the following form in the planewave basis $\{\psi_i = \frac{1}{\Omega}\exp(i(\mathbf{k}-\mathbf{G}_i))\}$, where $\{\mathbf{G}_i\}$ are reciprocal vectors.

$$\mathbf{H}_{ii} = \frac{(\mathbf{k}-\mathbf{G}_i)^2}{2} \tag{3.1}$$

$$\mathbf{H}_{ij} = V(\mathbf{G}_j - \mathbf{G}_i) \tag{3.2}$$

where the diagonal elements of $\mathbf{H}$ are kinetic energies of the planewaves in the basis and $V(\mathbf{G})$ is the Fourier component of the periodic pseudo potential with respect

to the reciprocal vector $\mathbf{G}$. In a realistic problem (Density Functional Theory based calculation, for instance), the eigenproblem of the Hamiltonian has to be solved self-consistently, which means the Hamiltonian itself (components of the potential energy) depends on the solutions of the problem (eigenwavefunctions and thus charge density distribution). To focus on the diagonalization technique itself, only the initial Hamiltonian built without the knowledge of charge density distribution is investigated in this report. In practical calculations, the situation can be much more complex since the self-consistent problem is essentially a nonlinear eigenproblem, which is beyond the scope of the course and far beyond the limited knowledge of the author. Most widely implemented algorithms in popular electronic structure calculation packages (such as Quantum ESPRESSO, SIESTA, etc.) are Davidson method and nonlinear conjugate gradient method[17], and the old wisdom in this field is that "Davidson is faster, while CG is more stable". To test and compare the performance of these algorithms, a specific type of non-linear CG algorithm (Teter-Payne-Allen, TPA)[17][18] is implemented. Besides common features shared among all non-linear CG flavors, TPA algorithm features an efficient update scheme (instead of common Rayleigh-Ritz type) and a smartly-designed preconditioner. After the *orthonormalized* conjugate gradient $\mathbf{r}_{cg}$ is computed at one iteration step, TPA parametrizes the new guess vector as

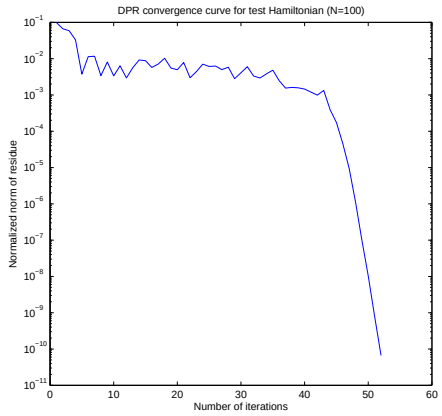
$$\mathbf{x}^{new} = \mathbf{x}^{old}\cos\theta + \mathbf{r}_{cg}\sin\theta \tag{3.3}$$

to maintain the unity of the guess eigenvector. Then the algorithm fits the energy functional (equivalent to Rayleigh quotient to be minimized) to the following functional form of θ

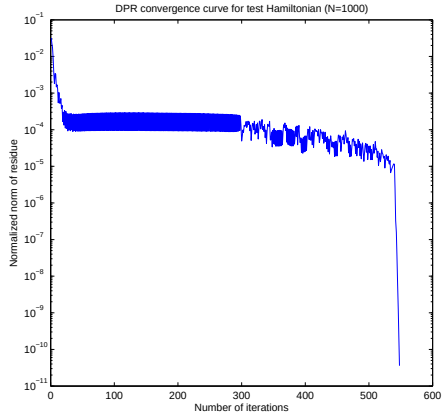
$$E(\theta) = E_{avg} + A_1\cos(2\theta) + B_1\sin(2\theta) \tag{3.4}$$

which turns out to work magically well in this specific type of problems. Then three function values (and/or the derivative values) of the energy functional at special points are evaluated to calculate the three unknown coefficients in equation (3.4), and the minimum point in terms of θ can be found analytically and thus used to update the guess vector in equation (3.3). Readers are referred to the original paper[18] for the detailed formulae. Compared to Block Davidson method, the non-linear CG can only solve eigenpairs one by one sequentially. In this report comparison will only be made in the case where the lowest eigenpair is of interest, while one has to keep in mind that since the cost of each iteration step of CG is cheaper than Davidson (especially when the subspace of Davidson grows relatively large), a more general discussion is necessary to give a full judgement. Limited by time and space, only the convergence behavior with respect to number of iteration steps will be discussed in this report.

So far the preconditioning issue has not been discussed. First we notice that the single-electron Hamiltonian in this problem exhibits a rather special structure of being "partially" diagonally dominant: diagonal elements corresponding to the kinetic energy of planewaves with large wavenumber overwhelm the off-diagonal elements whereas the ones corresponding to the low energy planewaves are actually comparable or even smaller than the off-diagonal elements. Since it is not diagonally dominant, original Davidson method (DPR) is not supposed to work super well especially when the dimension of the problem is large, which can be justified by figure 3.1. In the test, a Gaussian-type model pseudopotential is used and the calculation takes place at Γ point ($\mathbf{k} = 0$).



(a) N=100



(b) N=1000

Fig. 3.1: DPR does not work well when directly applied to the planewave Hamiltonian with $N = 1000$

Here the precondioner comes into play. TPA devised a specific preconditioner for planewave Hamiltonian

$$\mathbf{K}_{\mathbf{G},\mathbf{G}'} = \delta_{\mathbf{G},\mathbf{G}'} \frac{27 + 18\lambda + 12\lambda^2 + 8\lambda^3}{27 + 18\lambda + 12\lambda^2 + 8\lambda^3 + 16\lambda^4} \tag{3.5}$$

where $\lambda = \frac{(\mathbf{k}-\mathbf{G})^2/2}{T}$, and $T = \mathbf{x}^T\mathbf{D}\mathbf{x}$ is the kinetic energy of the current guess vector and $\mathbf{D}$ is the diagonal matrix corresponding to $\mathbf{H}$. The amazing properties of this preconditioner include that it is diagonal , that when $\|\mathbf{G}\|$ is large, $\mathbf{K}_{\mathbf{G},\mathbf{G}}$ approaches $1/(2(\lambda-1))$ with an asymptotic expansion correct to fourth order in $1/\lambda$, which is equivalent to Jacobi preconditioning for diagonal dominant elements, and that when $\|\mathbf{G}\|$ is small, $\mathbf{K}_{\mathbf{G},\mathbf{G}}$ approaches unity, keep the spectrum at low energies intact. To see how this preconditioner works, the result of a test run using CG with/without TPA preconditioning with the same initial guess is given in figure 3.2.

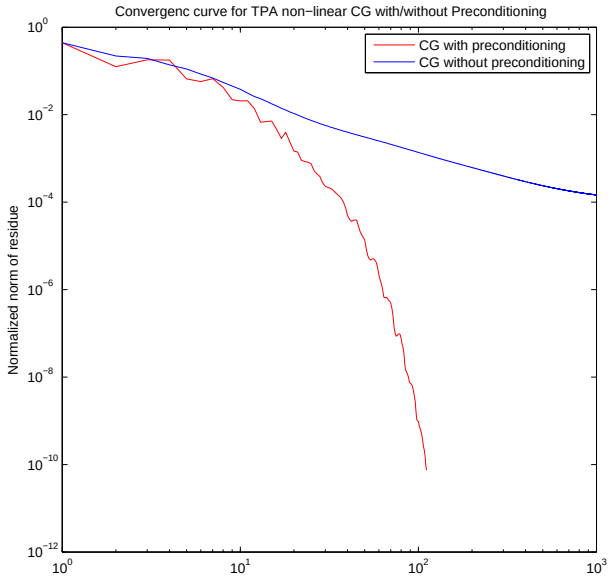


Fig. 3.2: Performance of non-linear CG gets improved a lot by preconditioning ($N = 1001$)

Given the previous discussions interpreting Davidson as a precondioned residue method, I became curious about what may happen if we combine the TPA preconditioner with the DPR method. Instead of using the original correction vector, I tried a new way of generating correction vectors as following

$$\delta = \mathbf{Kr} \tag{3.6}$$

And the result shows that this strategy seems to work magically well. Figure 3.3 shows that starting with the same initial guess vector, the number of iterations needed for TPA preconditioned DPR is around 20, while the original DPR seems to wander around for a long time before finally settling down. This example illustrates the possibility of improving performance of Davidson method by preconditioning in specific problems.

To conclude this section, a comparison between preconditioned Davidson and nonlinear CG when applied to the same (larger) Hamiltonian with the same starting vector is given in figure 3.4, which may not be really fair for CG.

4. Summary. This report mainly focuses on understanding the underlying mechanism that makes Davidson method work and reviewing different modifications and extensions of original DPR method. Different flavors of Davidson algorithm are implemented, so is the Blocked Davidson method. In a "not-so-realistic" toy problem, the possibility of improving Davidson method via preconditioning is explored, and the result compared with another state-of-the-art method, non-linear conjugate gradient algorithm (in TPA flavor). Furthur analysis is required to judge the performance of

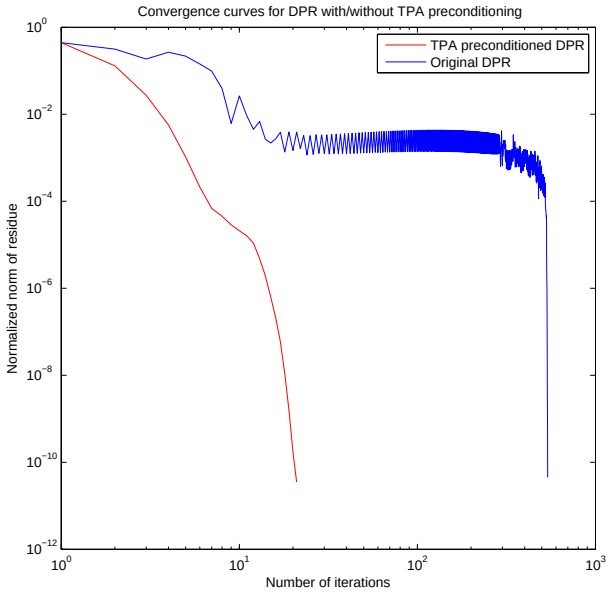


Fig. 3.3: Performance of DPR is improved significantly by TPA preconditioning ($N = 1001$)

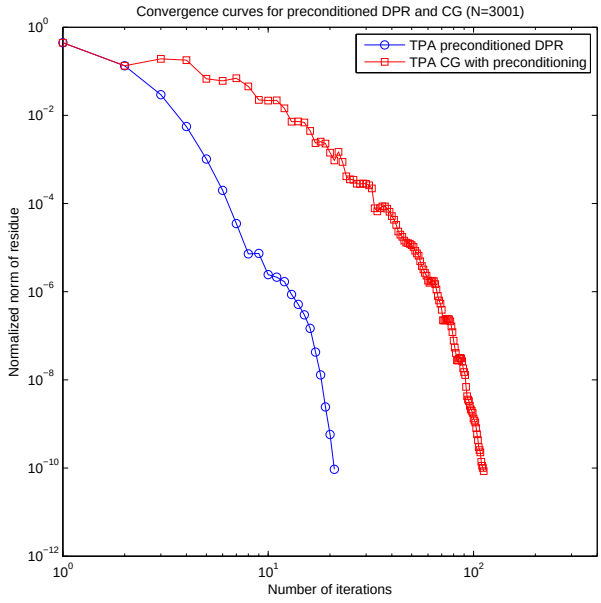


Fig. 3.4: Comparison between the convergence curves of preconditioned Davidson and non-linear CG

these two methods, and the result might as well depend on the specific problem. In realistic applications, the present problem needs to be solved self-consistently, which makes a totally different story.

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