
I.1.(b) Newton-type methods

1 Introduction

In this lecture, we will discuss methods based on Newton's method for solving large scale eigenvalue problems. The most well-known one is the Jacobi-Davidson method. We will start with the simple Newton's method for improving an approximation to an eigenpair. In this lecture we draw heavily from the Stewart's presentation¹.

2 Approximate Newton method

Suppose we have an approximate eigenpair (μ, z) of A , where z is a normalized vector, $\|z\|_2 = 1$, μ is the Rayleigh quotient corresponding to τ , $\mu = z^H A z$. Our objective is to find an improved approximation $(\mu + \eta, z + v)$ with the constraint $v \perp z$ (i.e., $v^H z = 0$).²

Newton correction formula. Let $(\mu + \eta, z + v)$ be an exact eigenpair of A

$$A(z + v) = (\mu + \eta)(z + v).$$

Then by the first-order approximation, we have the correction equation

$$(A - \mu I)v - \eta z = -r \quad \text{and} \quad z^H v = 0, \quad (2.1)$$

where r is the residual vector

$$r = Az - \mu z.$$

In matrix form, we have

$$\begin{pmatrix} A - \mu I & -z \\ z^H & 0 \end{pmatrix} \begin{pmatrix} v \\ \eta \end{pmatrix} = \begin{pmatrix} -r \\ 0 \end{pmatrix}$$

By the block elimination, we have the triangular system

$$\begin{pmatrix} A - \mu I & -z \\ 0 & z^H(A - \mu I)^{-1}z \end{pmatrix} \begin{pmatrix} v \\ \eta \end{pmatrix} = \begin{pmatrix} -r \\ z^H(A - \mu I)^{-1}r \end{pmatrix}$$

Hence, we have the following *Newton correction formula*

$$\eta = \frac{z^H(A - \mu I)^{-1}r}{z^H(A - \mu I)^{-1}z} \quad (2.2)$$

$$(A - \mu I)v = -r + \eta z \quad (2.3)$$

¹G. W. Stewart, *Matrix Algorithms, Volume II: Eigensystems*, SIAM, 2001 (Section 6.2).

²It is natural to require the correction v to be orthogonal to the approximate eigenvector z . For if $v \perp z$ and v is small compared with z , then a simple picture shows that the minimum distance between z and $\text{span}(z + v)$ is approximately $\|v\|_2$. In other words, v is close to the smallest possible correction.

Newton correction equation. An alternative to the Newton's correction formula (2.2) and (2.3) is to use a projection formulation. Let us rewrite the correction equation (2.1) as

$$(A - \mu I)v = -r + \eta z \quad \text{and} \quad z^H v = 0. \quad (2.4)$$

Let

$$P = I - zz^H$$

be the orthogonal projector onto the orthogonal complement of z . Then it is easy to verify that

1. $Pz = 0$,
2. $Pv = v$,
3. $Pr = r$.

Consequently, the correction equation (2.4) can be written as

$$P(A - \mu I)Pv = -r \quad \text{and} \quad v \perp z.$$

or

$$(I - zz^H)(A - \mu I)(I - zz^H)v = -r \quad \text{and} \quad v \perp z. \quad (2.5)$$

We will call (2.5) the **Newton correction equation**.

Theorem 2.1. *v satisfies (2.2) and (2.3) if and only if v satisfies (2.5).*

Proof. We have already shown that if v satisfies (2.2) and (2.3), then v satisfies (2.5). Suppose v satisfies (2.5). Then

$$(A - \mu I)(I - zz^H)v = -r + zz^H(A - \mu I)(I - zz^H)v = -r + \alpha z$$

and

$$v = -(A - \mu I)^{-1}r + \alpha(A - \mu I)^{-1}z.$$

Since $z^H v = 0$, we have

$$\alpha = \frac{z^H(A - \mu I)^{-1}r}{z^H(A - \mu I)^{-1}z} = \eta.$$

Thus v satisfies (2.2) and (2.3). □

Although the Newton correction equation (2.5) does not give the correction explicitly, it offers an opportunity to apply an iterative method to solve the correction equation, which in turn we need only to compute the matrix-vector product $P(A - \mu I)Py$, where y is an arbitrary vector, something that is easily done. We will return to this at the end of this lecture.

3 Jacobi-Davidson method

Jacobi-Davidson method is a combination of the Newton correction equation and Rayleigh-Ritz approximations. Therefore, it might be better called the **Newton-Rayleigh-Ritz method**.

3.1 Basic Jacobi-Davidson method

We start with the basic Jacobi-Davidson method to compute only one eigenpair whose eigenvalue is near a focal point τ . The following pseudo-code is a combination of a combination of the Newton correction equation and Rayleigh-Ritz approximations. The starting vector v is normalized, $\|v\|_2 = 1$.

Algorithm 3.1 (The basic Jacobi-Davidson algorithm).

1. $V = v$;
2. for $k = 1, 2, \dots, k_{\max}$
3. Using V compute a normalized Ritz pair (μ, z) such that μ is near τ ;
4. $r = Az - \mu z$;
5. if r is sufficiently small, return (μ, z) , exit;
6. choose a shift κ near τ or μ ;
7. solve the correction equation
 $(I - zz^H)(A - \kappa I)(I - zz^H)v = -r$ and $v^H z = 0$;
8. orthonormalize v with respect to V ;
9. $V = \begin{pmatrix} V & v \end{pmatrix}$;
10. end for
11. signal nonconvergence.

The algorithm has two parameters: τ and κ . τ is the center of a focal region in which we wish to find an eigenpair, and κ is generally chosen equal to τ or μ . However, if it is inexpensive to vary κ , then it can be shown that by choosing $\kappa = \mu$, the algorithm converges quadratically.

The Jacobi-Davidson method can be viewed as an improvement of Davidson's algorithm, which builds up a correction subspace as shown below. The chief difference is in the correction equation, which is essentially an approximate inverse power method. The lack of orthogonality of the correction vector v to the approximate eigenvector v is a drawback. Jacobi-Davidson method was originally derived by extending an algorithm of Jacobi for approximating eigenvectors of diagonally dominant matrices.

Algorithm 3.2 (Davidson's method for the smallest eigenvalue).

1. $V = v$;
2. for $k = 1, 2, \dots, k_{\max}$
3. Using V to compute the Ritz pair (μ, z) , where μ is the smallest eigenvalues of the Rayleigh quotient;
4. $r = Az - \mu z$;
5. if r is sufficiently small, return (μ, z) , exit;
6. solve the system $(D - \mu I)v = r$;
7. $v = Pv / \|Pv\|_2$, where $P = I - VV^H$;
8. $V = \begin{pmatrix} V & v \end{pmatrix}$;
9. end for
10. signal nonconvergence.

3.2 Extended Jacobi-Davidson method

The basic Jacobi-Davidson method is for computing only one eigenpair. We now show how to extend the method for computing multiple eigenpairs. Without loss of generality, we assume that we have computed a partial Schur decomposition

$$AU = UT, \tag{3.1}$$

Our goal now is to extend the partial Schur decomposition of A of one order higher:

$$A \begin{pmatrix} U & u \end{pmatrix} = \begin{pmatrix} U & u \end{pmatrix} \begin{pmatrix} T & t \\ 0 & \mu \end{pmatrix} \quad (3.2)$$

Let us begin with the Schur reduction process as we have learned to prove the existence of Schur decomposition. Assume $\begin{pmatrix} U & U_\perp \end{pmatrix}$ is unitary and write

$$\begin{pmatrix} U^H \\ U_\perp^H \end{pmatrix} A \begin{pmatrix} U & U_\perp \end{pmatrix} = \begin{pmatrix} U^H A U & U^H A U_\perp \\ U_\perp^H A U & U_\perp^H A U_\perp \end{pmatrix} \equiv \begin{pmatrix} T & H \\ 0 & B \end{pmatrix}. \quad (3.3)$$

Let (μ, z) be a normalized eigenpair of B , and let $\begin{pmatrix} z & Z_\perp \end{pmatrix}$ be unitary. Then

$$\begin{pmatrix} z^H \\ Z_\perp^H \end{pmatrix} B \begin{pmatrix} z & Z_\perp \end{pmatrix} = \begin{pmatrix} z^H B z & z^H B Z_\perp \\ Z_\perp^H B z & Z_\perp^H B Z_\perp \end{pmatrix} \equiv \begin{pmatrix} \mu & g^H \\ 0 & C \end{pmatrix}. \quad (3.4)$$

By combining (3.3) and (3.4), we have

$$\begin{pmatrix} U^H \\ (U_\perp z)^H \\ (U_\perp Z_\perp)^H \end{pmatrix} A \begin{pmatrix} U & U_\perp z & U_\perp Z_\perp \end{pmatrix} = \begin{pmatrix} T & Hz & HZ_\perp \\ 0 & \mu & g^H \\ 0 & 0 & C \end{pmatrix}.$$

Hence

$$A \begin{pmatrix} U & U_\perp z \end{pmatrix} = \begin{pmatrix} U & U_\perp z \end{pmatrix} \begin{pmatrix} T & Hz \\ 0 & \mu \end{pmatrix}$$

is a partial Schur decomposition of A of one order higher than (3.1).

Now it is clear how to extend the partial Schur decomposition. However, this dense matrix process is not suitable for large sparse problems. In this case, we need to use the projection formulation. Let $P = U_\perp U_\perp^H = I - U U^H$ be the orthogonal projection onto the column subspace of U_\perp . Let

$$A_\perp = P A P.$$

Then it is easy to verify that

$$A_\perp = U_\perp B U_\perp^H.$$

The following lemma shows the one-to-one correspondence between an eigenpair of A_\perp and B .

Lemma 3.1.

- (a) If (μ, z) is an eigenpair of B , then $(\mu, y) = (\mu, U_\perp z)$ is an eigenpair of A_\perp and $y \perp U$.
- (b) If (μ, y) is an eigenpair of A_\perp and $y \perp U$, then $(\mu, z) = (\mu, U_\perp^H y)$ is an eigenpair of B .

Proof. Both results can be verified directly. For (a), if (μ, z) is an eigenpair of B , then

$$A_\perp y = U_\perp B U_\perp^H U_\perp z = U_\perp B z = U_\perp (\mu z) = \mu y$$

and $y^H U = z^H U_\perp^H U = 0$. Hence $(\mu, y) = (\mu, U_\perp z)$ is an eigenpair of A_\perp and $y \perp U$.

For (b), if (μ, y) is an eigenpair of A_\perp and $y \perp U$, then

$$\begin{aligned} B z &= (U_\perp^H A U_\perp)(U_\perp^H y) \\ &= U_\perp^H U_\perp (U_\perp^H A U_\perp)(U_\perp^H y) \\ &= U_\perp^H P A P y \\ &= U_\perp^H A_\perp y \\ &= U_\perp^H (\mu y) \\ &= \mu U_\perp^H y \\ &= \mu z. \end{aligned}$$

Hence, $(\mu, z) = (\mu, U_\perp^H y)$ is an eigenpair of B . □

By Lemma 3.1, our computational task is now turned into solving a normalized eigenpair (μ, y) satisfying

$$A_{\perp} y = \mu y \quad \text{and} \quad y \perp U. \quad (3.5)$$

Once we have found a normalized eigenpair (μ, y) of (3.5), an extended Schur decomposition is given by

$$A \begin{pmatrix} U & y \end{pmatrix} = \begin{pmatrix} U & y \end{pmatrix} \begin{pmatrix} T & t \\ 0 & \mu \end{pmatrix},$$

where

$$t = U^H A y.$$

To solve the eigenvalue problem (3.5), we can use the Jacobi-Davidson procedure. Assume that after computing the partial Schur decomposition (3.1), we have an orthonormal matrix V of corrections, a new correction vector v , and V and v are orthogonal to U . Then we proceed the following steps:

1. Orthogonalize v with respect to V and update $V = \begin{pmatrix} V & v \end{pmatrix}$.
2. Compute the Rayleigh quotient $C = V^T A_{\perp} V = V^T A V$, since V is orthogonal to U .
3. Compute an eigenpair (μ, p) of C , which gives the Ritz pair $(\mu, z) = (\mu, Vp)$ as an approximate eigenpair of A .
4. Compute the residual for testing convergence.

$$r = A_{\perp} z - \mu z$$

5. Solve the correction equation

$$(I - z z^H) A_{\perp} (I - z z^H) v = -r \quad \text{and} \quad v \perp U z. \quad (3.6)$$

to get another correction to be added to V .

REMARK 3.1. In the statement 4, to be exact, we should test the residual of the Ritz pair (μ, z) with respect to A ,

$$s = A z - U t - \mu z$$

where $t = U^H A V p$. To assess the size of s , we compute the size of its components in U and U_{\perp} . First, multiplying s by U^H , we get

$$U^H s = U^H A z - U^H U t - \mu U^H z = U^H A V p - U^H U t - \mu U^H V p = t - t - 0 = 0.$$

Hence $P s = U U^H s = 0$. On the other hand, if we multiply s by $P_{\perp} = U_{\perp} U_{\perp}^H = I - U U^H$, we get

$$\begin{aligned} P_{\perp} s &= U_{\perp} U_{\perp}^H s = (I - U U^H) s \\ &= (I - U U^H) A (I - U U^H) z - (I - U U^H) U t - \mu (I - U U^H) z \\ &= (I - U U^H) A (I - U U^H) z - \mu z \\ &= P_{\perp} A P_{\perp} z - \mu z = r. \end{aligned}$$

It follows that $\|s\|_2 = \|(P + P_{\perp})s\|_2 = \|P_{\perp} s\|_2 = \|r\|_2$.

The following algorithm implements this scheme. The inputs, in addition to U , are an $n \times (\ell - 1)$ matrix V of orthonormalized correction vectors, an additional correction vector v , $W = A V$, $C = V^H W$, and a focal point τ .

Algorithm 3.3 (Extended Jacobi-Davidson algorithm).

1. for $k = \ell$ to m
2. orthonormalize v with respect to U and V ;
3. $w = Av$;
4. $C = \begin{pmatrix} C & V^H w \\ v^H w & v^H W \end{pmatrix}$;
5. $V = \begin{pmatrix} V & v \end{pmatrix}$ and $W = \begin{pmatrix} W & w \end{pmatrix}$;
6. find an eigenpair (μ, p) of C such that μ is nearest τ ;
7. $z = Vp$;
8. $y = Wp$;
9. $r = y - \mu z$;
10. orthogonalize r with respect to U ;
11. if r is sufficiently small, return $u = z$, $t = U^H y$ and μ , exit;
12. choose a shift κ near τ or μ ;
13. solve the correction equation;
 $(I - zz^H)(A_\perp - \kappa I)(I - zz^H)v = -r$ and $v \perp U$ and $v \perp z$;
14. endfor
15. return v .

Restarting. The Jacobi-Davidson algorithm builds up a basis V from which eigenvectors can be extracted by the Rayleigh-Ritz method. Ultimately, V will become so large that it exceeds the storage capacity. At this point, we must restart with a reduced basis. The following is a **Schur-Rayleigh-Ritz process** for the basis reduction:

1. Compute the Schur decomposition $C = QTQ^H$, where the diagonal entries of T are ordered such that $|t_{ii} - \tau| \leq |t_{i+1,i+1} - \tau|$;
2. Determine the largest integer ℓ such that $|t_{\ell,\ell} - \tau| \leq \rho$;
3. $V = VQ[:, 1 : \ell]$;
4. $W = WQ[:, 1 : \ell]$;
5. $C = Q[:, 1 : \ell]^H C Q[:, 1 : \ell]$.

As a result, we replace V with a basis for the primitive Ritz subspace corresponding to the Ritz values close to the focal point τ .

Solving the correction equation. If we take $Q = z$ or $Q = \begin{pmatrix} U & z \end{pmatrix}$, then the correction equations (2.5) and (3.6) can be written as

$$(I - QQ^H)(A - \kappa I)(I - QQ^H)v = -r \quad \text{and} \quad v, r \perp Q \quad (3.7)$$

Since $v \perp Q$, we have

$$(I - QQ^H)(A - \kappa I)v = -r,$$

or

$$(A - \kappa I)v = -r + QQ^H(A - \kappa I)v.$$

Hence

$$v = -(A - \kappa I)^{-1}r + (A - \kappa I)^{-1}QQ^H(A - \kappa I)v.$$

Since $Q^H v = 0$, we have

$$0 = Q^H v = -Q^H(A - \kappa I)^{-1}r + Q^H(A - \kappa I)^{-1}QQ^H(A - \kappa I)v,$$

or

$$Q^H(A - \kappa I)^{-1}Q(Q^H(A - \kappa I)v) = Q^H(A - \kappa I)^{-1}r.$$

Hence we have the following scheme to solve the correction equation (3.7) exactly.

1. Compute $F = (A - \kappa I)^{-1}Q$;
2. Compute $C = Q^H F$;
3. Solve $(A - \kappa I)x = r$ for x ;
4. Compute $b = Q^H x$;
5. Solve $Ca = b$ for a ;
6. $v = -x + Fa$.

The above scheme suggests that we should avoid ill-conditioning in $A - \kappa I$. This means we should avoid a focal point that accurately approximates an eigenvalue λ of A . Even though such a focal point will speed up convergence to λ , it could retard convergence to other eigenvalues.

For large sparse problem, we can use an iterative method to solve the correction equation (3.7). To use a Krylov iterative method, we only need to be able to form the matrix-vector product $(I - QQ^H)(A - \kappa I)(I - QQ^H)w$ for an arbitrary vector w , which can be easily done. In practice, as we know that the convergence of an iterative method can improved, often dramatically, by using a proper *preconditioning*. Let the preconditioner M is determined from $A - \kappa I$. Then to approximate the projected system, M must also be projected. Therefore, the matrix-vector product will be performed by the following two steps:

1. Compute $y = (I - QQ^H)(A - \kappa I)(I - QQ^H)w$;
2. Solve $(I - QQ^H)M(I - QQ^H)x = y$, where $y, x \perp Q$.

The system in Statement 2 can be solved use the above exact solver. The use of a preconditioned solver gives us more freedom to choose a shift κ . (1) The system to be solved involves the preconditioner M , not the shifted matrix. Thus if we can find an effective preconditioner that does not depend on κ , we can vary κ . (2) We can place κ near an eigenvalue, since we work only with the projected matrix $(I - QQ^H)(A - \kappa I)(I - QQ^H)$ and never have to explicitly solve systems involving $A - \kappa I$. (3) We can choose to solve correction equations more or less accurately. Unfortunately, there is very little hard analysis to guide us in this matter. There is a tension between the local convergence driven by the Newton iteration and the broader convergence driven by the correction subspace. From a local point of view, only a certain number of figures of v accurately contribute to the improvement of z , and there is no reason to solve the correction equation too accurately.

4 Further reading

The following work by Peters and Wilkinson presents the Newton's method and its relation to the inverse power method for eigenvalue problem:

- G. Peters and J. H. Wilkinson, Inverse iteration, ill-conditioned equations and Newton's method. SIAM Review, 21;339-360, 1979.

The Jacobi-Davidson method was proposed in 1996 by extending algorithm of Jacobi for approximating eigenvectors of diagonally dominant matrices. Their major contributions was the introduction of the correction equation, which expresses the correction in terms of a projection of the original matrix. It is the key to make the method effective for large sparse matrices,

- G. L. G. Sleijpen and H. A. van der Vorst, A Jacobi-Davidson iteration method for linear eigenvalue problems. SIAM J. on Matrix Analysis and Applications, 17:401-425, 1996.

Algorithmic templates of Jacobi-Davidson methods by Sleijpen and van der Vorst can be found in sections 4.7, 5.6, 7.12 and 8.4 of the following book:

- Z. Bai, J. Demmel, J. Dongarra, A. Ruhe and H. A. van der Vorst (editors), Templates for the Solution of Algebraic Eigenvalue Problems: A Practical Guide. SIAM, 2000.

Recent development includes

- A. Stathopoulos, Nearly optimal preconditioned methods for Hermitian eigenproblems under limited memory. Part I: Seeking one eigenvalue, SIAM J. Sci. Comput., 29:481–514, 2007
- A. Stathopoulos and J. R. McCombs, Nearly optimal preconditioned methods for Hermitian eigenproblems under limited memory. Part II: Seeking many eigenvalues, SIAM J. Sci. Comput., 29:2162-2188, 2007
- H. Voss, A Jacobi-Davidson method for nonlinear and nonsymmetric eigenproblems, Computers and Structures, 85:1284-1292, 2007
- J. Rommes, Arnoldi and Jacobi-Davidson methods for generalized eigenvalue problems $Ax = \lambda Bx$ with singular B , Math. Comp, 77:995-1015, 2008.