CHAPTER 3 : JACOBI–DAVIDSON METHOD

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Davidson Method

The Davidson method is a popular technique to compute a few of the smallest (or largest) eigenvalues of a large sparse real symmetric matrix.

It is effective when the matrix is nearly diagonal, i.e. if the matrix of eigenvectors is close to the identity matrix. It is mainly used for problems of theoretical chemistry (ab initio calculations in quantum chemistry) where the matrices are strongly diagonally dominant.

Similar to the Lanczos method Davidson's method is an iterative projection method which however does not take advantage of Krylov subspaces but uses the Rayleigh–Ritz procedure with non-Krylov spaces and expands the search spaces in a different way.

Davidson method

Let $U_k := [u^1, \ldots, u^k] \in \mathbb{R}^{(n,k)}$ be a matrix with orthonormal columns, and let (θ, s) be an eigenpair of the projected problem

$$U_k^H A U_k s = \lambda\, s,$$

and $y = U_k s$.

Davidson (1975) suggested to expand the ansatz space span U_k by the direction

$$t := (D_A - \theta I)^{-1} r$$

where $r := Ay - \theta y$ is the residual of the Ritz pair (y, θ) and D_A denotes the diagonal of A. u^{k+1} is obtained by orthogonalizing t against U_k.

A little irritating is the fact that the method fails for diagonal matrices: if A is diagonal and (θ, y) is a Ritz pair then

$$t = (D_A - \theta I)^{-1} r = y \in \operatorname{span} U_j,$$

and the space span U_j will not be not expanded.

Davidson Algorithm

Choose initial vector u^1 with $\|u^1\| = 1$, $U_1 = [u^1]$
for $j = 1, 2, \ldots$ **do**
  $w^j = Au^j$
  for $k = 1, \ldots, j-1$ **do**
    $b_{kj} = (u^k)^H w^j$
    $b_{jk} = (u^j)^H w^k$
  end for
  $b_{jj} = (u^j)^H w^j$
  Compute largest eigenvalue θ of B
  and corresponding eigenvector s with $\|s\| = 1$
  $y = U_j s$
  $r = Ay - \theta y$
  $t = (D_A - \theta I)^{-1} r$
  $t = t - U_j U_j^H t$
  $u^{j+1} = t/\|t\|$
  $U_{j+1} = [U_j, u^{j+1}]$
end for

Jacobi's method

In addition to the well known method for determining all eigenvalues (and eigenvectors) of a symmetric matrix Jacobi suggested the following method for improving known eigenvalue–eigenvector approximations.

Assume that A is diagonally dominant, and let $\alpha := a_{11}$ be the maximum diagonal element. Then α is an approximation to the maximum eigenvalue and e^1 an approximation to the corresponding eigenvector.

To improve these approximations we have to solve the problem

$$A \begin{pmatrix} 1 \\ z \end{pmatrix} = \begin{pmatrix} \alpha & c^T \\ b & F \end{pmatrix} \begin{pmatrix} 1 \\ z \end{pmatrix} = \lambda \begin{pmatrix} 1 \\ z \end{pmatrix}.$$

The eigenproblem is equivalent

$$\begin{aligned} \lambda &= \alpha + c^T z \\ (F - \lambda I) z &= -b. \end{aligned}$$

Jacobi's method ct.

Jacobi suggested to solve this problem iteratively:

$$\begin{aligned} \theta_k &= \alpha + c^T z_k \\ (D - \theta_k I) z_{k+1} &= (D - F) z_k - b, \end{aligned}$$

where D denotes the diagonal of F.

Sleijpen & van der Vorst (1996) suggested to combine the approach of Davidson and the improvement of Jacobi in an iterative projection method, i.e. given a Ritz pair (θ, u) corresponding to some subspace $\mathcal{U}$ to expand $\mathcal{U}$ by a direction which is orthogonal to u and satisfies (approximately) a correction equation.

Jacobi–Davidson method

Let u be an approximation to an eigenvector of A, and let θ be the Ritz value corresponding to u. Similarly to Jacobi's approach we determine an improvement of u which is orthogonal to u.

If $\| u\| = 1$ then the orthogonal projection of the matrix A to $u^\perp$ reads

$$B = (I - uu^H) A (I - uu^H).$$

From $\theta = u^H A u$ one gets

$$A = B + Auu^H + uu^H A - \theta uu^H.$$

An eigenvalue-eigenvector pair (λ, x), $x = u + v$, $v \perp u$ satisfies

$$A(u + v) = \lambda(u + v),$$

and from $Bu = 0$ it follows

$$(B - \lambda I) v = -r + (\lambda - \theta - u^H A v) u$$

where $r = Au - \theta u$.

Jacobi–Davidson method ct.

By the orthogonality of $(B - \lambda I)v$ and u and of r and u it follows that $\lambda - \theta - u^H A v = 0$, and therefore the improvement v satisfies

$$(B - \lambda I) v = -r = (A - \theta I) u.$$

Since λ is not known we replace it by the Ritz value θ (or if θ is not yet close to a wanted eigenvalue we replace it by a target value in the vicinity of which we are looking for eigenvalues) to obtain the correction equation

$$(I - uu^H)(A - \theta I)(I - uu^H) v = -r.$$

We expand the search space which yielded the Ritz pair (θ, u) by the solution of the correction equation, and determine with this expanded search space the next Ritz pair.

This is the basis of the Jacobi-Davidson method introduced by Sleijpen and van der Vorst 1996.

Jacobi–Davidson method ct.

$v \in u^\perp$ yields $(I - uu^H)v = v$. Hence, the correction equation can be rewritten as

$$(A - \theta I)v = -r + \alpha u,$$

where $\alpha \in \mathbb{C}$ has to be determined such that $v \perp u$.

This implies

$$\begin{aligned} v &= -(A-\theta I)^{-1} r + \alpha (A-\theta I)^{-1} u \\ &= -u + \alpha (A-\theta I)^{-1} u \end{aligned}$$

Since the search space is expanded by v and since u is already contained in the current search space, the new search space will contain in particular the vector $t := (A - \theta I)^{-1} u$.

t is the improvement of the Ritz pair (θ, u) by one step of inverse iteration with shift θ and initial vector u. Hence, the Jacobi-Davidson method can be considered as an acceleration of inverse iteration, and can be expected to converge at least as fast as inverse iteration (i.e. quadratic or even cubic).

Jacobi–Davidson method ct.

It is a disadvantage of the Jacobi–Davidson method that in every step one has to solve a linear system with varying coefficient matrix $A - \theta I$.

It was observed that fast convergence was maintained if the correction equation was solved only approximately.

Sleijpen and van der Vorst suggest to use MINRES if A is symmetric and GMRES or BiCGStab otherwise and to use a suitable preconditioner K for $A - \theta I$ in any case.

Every other approximate method is fine if only the projector $I - uu^H$ is taken account for.

A different motivation, V. 2006

Given a search space $\mathcal{V} \subset \mathbb{C}^n$. Expand $\mathcal{V}$ by a direction such that the expanded space has a high approximation potential for the next wanted eigenvector.

Let the columns of V form an orthonormal basis of $\mathcal{V}$, and let θ be an eigenvalue of the projected problem

$$V^H A V y = \lambda y$$

and $x = Vy$, $\|x\| = 1$ a corresponding Ritz vector.

Because of its good approximation property we want to expand the search space by the direction of Rayleigh quotient iteration
$v = (A - \theta I)^{-1} x / \|(A - \theta I)^{-1} x\|$.

However, in a truly large problem the vector v will not be accessible but only an inexact solution $\tilde{v} := v + e$ of $(A - \theta I)v = x$, and the next iterate will be a solution of the projection of $Ax = \lambda x$ onto the space $\tilde{\mathcal{V}} := \mathrm{span}\{\mathcal{V}, \tilde{v}\}$.

Expansion of search space

We assume that x is already a good approximation to an eigenvector of A. Then v will be an even better approximation, and therefore the eigenvector we are looking for will be very close to the plane $E := \mathrm{span}\{x, v\}$.

We therefore neglect the influence of the orthogonal complement of x in $\mathcal{V}$ on the next iterate and discuss the nearness of the planes E and $\tilde{E} := \mathrm{span}\{x, \tilde{v}\}$.

If the angle between these two planes is small, then the projection of $Ax = \lambda x$ onto $\tilde{\mathcal{V}}$ should be similar to the one onto $\mathrm{span}\{\mathcal{V}, v\}$, and the approximation properties of inverse iteration should be maintained.

If this angle can become large, then it is not surprising that the convergence properties of inverse iteration are not reflected by the projection method.

Theorem

Let $\phi_0 = \arccos(x^T v)$ denote the angle between x and v, and the relative error of $\tilde{v}$ by $\varepsilon := \|e\|$.

Then the maximal possible acute angle between the planes E and $\tilde{E}$ is

$$\beta(\varepsilon) = \begin{cases} \arccos\sqrt{1-\varepsilon^2/\sin^2\phi_0} & \text{if} \quad \varepsilon \le |\sin\phi_0| \\ \frac{\pi}{2} & \text{if} \quad \varepsilon \ge |\sin\phi_0| \end{cases}$$

Proof

For $\varepsilon > |\sin\phi_0|$ the vector x is contained in the ball with center v and radius ε, and therefore the maximum acute angle between E and $\tilde{E}$ is $\frac{\pi}{2}$.

For $\varepsilon \le |\sin\phi_0|$ we assume without loss of generality that $v = (1,0,0)^T$, $\tilde{v} = (1+e_1, e_2, e_3)^H$, and $x = (\cos\phi_0, \sin\phi_0, 0)^T$.

Obviously the angle between E and $\tilde{E}$ is maximal, if the plane $\tilde{E}$ is tangential to the ball B with center v and radius ε.

Then $\tilde{v}$ is the common point of ∂B and the plane $\tilde{E}$, i.e. the normal vector $\tilde{n}$ of $\tilde{E}$ has the same direction as the perturbation vector e:

An easy calculation now yields the stated formula:

Proof ct.

$$e = \begin{pmatrix} e_1 \\ e_2 \\ e_3 \end{pmatrix} = \gamma\tilde{n} = \gamma \begin{pmatrix} \cos\phi_0 \\ \sin\phi_0 \\ 0 \end{pmatrix} \times \begin{pmatrix} 1+e_1 \\ e_2 \\ e_3 \end{pmatrix} = \gamma \begin{pmatrix} e_3\sin\phi_0 \\ -e_3\cos\phi_0 \\ e_2\cos\phi_0 - (1+e_1)\sin\phi_0 \end{pmatrix}.$$

Hence, we have

$$e_1 = \gamma\sin\phi_0 e_3, \quad e_2 = -\gamma\cos\phi_0 e_3,$$

and the third component yields

$$\begin{aligned} e_3 &= \gamma(-\gamma\cos^2\phi_0 e_3 - (1+\gamma\sin\phi_0 e_3)\sin\phi_0) \\ &= -\gamma^2 e_3 - \gamma\sin\phi_0, \end{aligned}$$

i.e.

$$e_3 = -\frac{\gamma}{1+\gamma^2}\sin\phi_0. \quad (1)$$

Proof ct.

Moreover, from

$$\varepsilon^2 = e_1^2 + e_2^2 + e_3^2 = \gamma^2\sin^2\phi_0 e_3^2 + \gamma^2\cos^2\phi_0 e_3^2 + e_3^2 = (1+\gamma^2)e_3^2,$$

we obtain

$$\varepsilon^2 = \frac{\gamma^2}{1+\gamma^2}\sin^2\phi_0, \quad \text{i.e. } \gamma^2 = \frac{\varepsilon^2}{\sin^2\phi_0 - \varepsilon^2}.$$

Inserting into equation (1) yields

$$e_3^2 = \frac{1}{1+\gamma^2}\varepsilon^2 = \Big(1 - \frac{\varepsilon^2}{\sin^2\phi_0}\Big)\varepsilon^2,$$

and since the normal vector of E is $n = (0,0,1)^T$, we finally get

$$\cos\beta(\varepsilon) = \frac{e^T n}{\|n\|\cdot\|e\|} = \frac{e_3}{\varepsilon} = \sqrt{1 - \frac{\varepsilon^2}{\sin^2\phi_0}}. \quad \square$$

Expansion by inexact inverse iteration

Obviously for every $\alpha \in \mathbb{R}$, $\alpha \neq 0$ the plane E is also spanned by x and $x + \alpha v$.

If $\tilde{E}(\alpha)$ is the plane which is spanned by x and a perturbed realization $x + \alpha v + e$ of $x + \alpha v$ then by the same arguments as in the proof of the Theorem the maximum angle between E and $\tilde{E}(\alpha)$ is

$$\gamma(\alpha, \varepsilon) = \begin{cases} \arccos \sqrt{1 - \varepsilon^2 / \sin^2 \phi(\alpha)} & \text{if} \quad \varepsilon \leq |\sin \phi(\alpha)| \\ \frac{\pi}{2} & \text{if} \quad \varepsilon \geq |\sin \phi(\alpha)| \end{cases}$$

where $\phi(\alpha)$ denotes the angle between x and $x + \alpha v$.

Since the mapping

$$\phi \mapsto \arccos \sqrt{1 - \varepsilon^2 / \sin^2 \phi}$$

decreases monotonically the expansion of the search space by an inexact realization of $t := x + \alpha v$ is most robust with respect to small perturbations, if α is chosen such that x and $x + \alpha v$ are orthogonal

Expansion by inexact inverse iteration

$x^T(x + \alpha v) = 0$ if and only if

$$t = x - \frac{x^H x}{x^H (A - \theta I)^{-1} x} (A - \theta I)^{-1} x. \qquad (*)$$

which is the solution of the correction equation

$$(I - xx^H)(A - \theta I)(I - xx^H)t = (A - \theta I)x, \quad t \perp x.$$

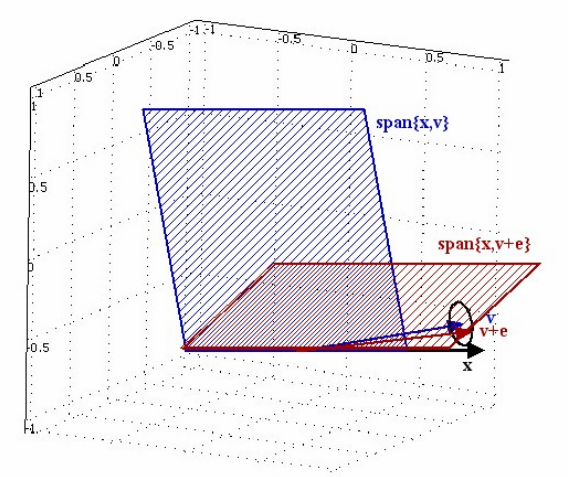
of the Jacobi–Davidson method.

Hence, the Jacobi–Davidson method is the most robust realization of an expansion of a search space such that the direction of inverse iteration is contained in the expanded space in the sense that it is least sensitive to inexact solves of linear systems $(A - \theta I)v = x$.

The maximum acute angle between E and $\tilde{E}(\alpha)$ satisfies

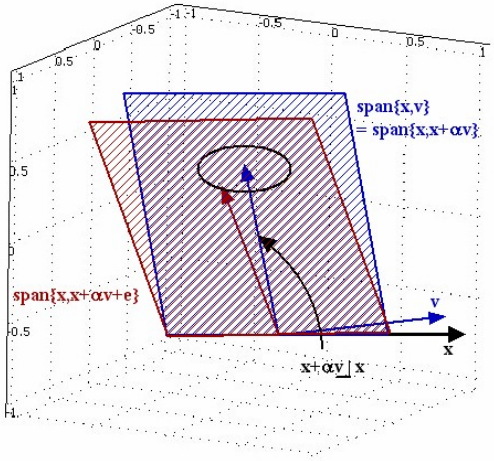
$$\gamma(\alpha, \varepsilon) = \begin{cases} \arccos \sqrt{1 - \varepsilon^2} & \text{if} \quad \varepsilon \leq 1 \\ \frac{\pi}{2} & \text{if} \quad \varepsilon \geq 1 \end{cases}.$$

Inexact inverse iteration



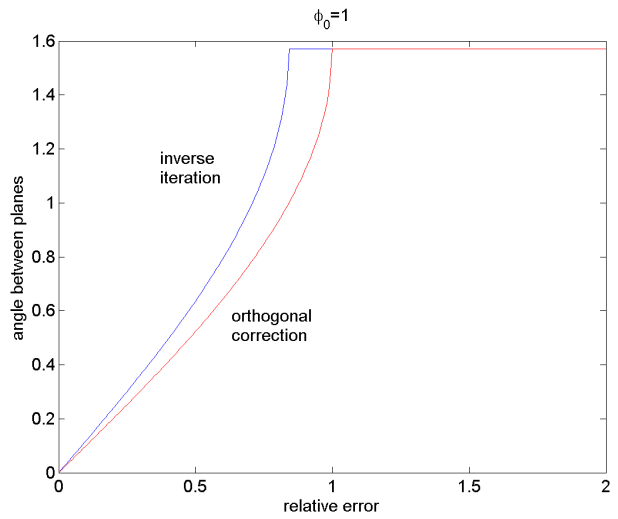
For truly large problems v is not available, but has to be replaced by an inexact solution $v + e$ of $(A - \theta I)v = x$.

Orthogonal expansion

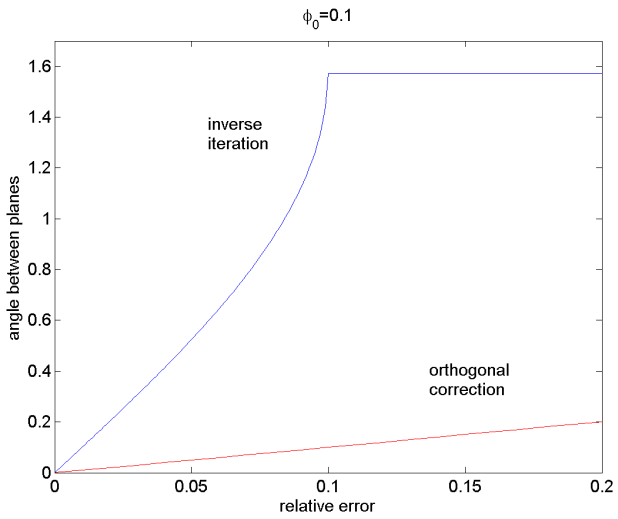


$\text{span}\{x, x + \alpha v\}$, α such that $x^T(x + \alpha v) = 0$ is more robust to perturbations $\text{span}\{x, x + \alpha v + e\}$ than $\text{span}\{x, v\}$.

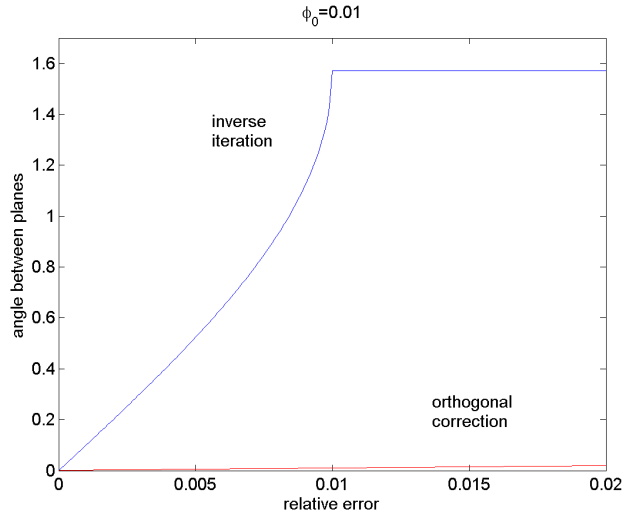
Expansion by inexact inverse iteration ct.



Expansion by inexact inverse iteration ct.



Expansion by inexact inverse iteration ct.



Subspace extraction

Projection methods usually yield good approximations to extreme eigenvalues, but often they do not work well if one is interested in interior eigenvalues.

The reason is that Ritz values converge 'monotonically' to exterior eigenvalues. A Ritz value that is close to a target value in the interior of the spectrum may be on its way to some exterior eigenvalue, and the corresponding Ritz vector may have a small components in the directions of eigenvectors close to the target value. Clearly such a Ritz vector is a poor candidate for search space expansion or restart.

Example

$$A = \mathrm{diag}\{1,2,3\},\ x = (1,0,1)^T \quad \Longrightarrow \quad R_A(x) = 2 = \lambda_2.$$

$R_A(x)$ is an eigenvalue of A, but x is far away from being a corresponding eigenvector.

For interior eigenvalues Rayleigh–Ritz generally gives poor approximate eigenvectors.

Harmonic Ritz values/vectors (Morgan 1991)

If eigenvalues close to some τ are desired, consider Ritz values of $(A-\tau I)^{-1}$ with respect to some subspace $\mathcal{W} = \operatorname{span}(W)$:

$$W^H(A-\tau I)^{-1}Wz = \frac{1}{\theta-\tau}W^HWz$$

To avoid the inverse matrix, choose $W := (A-\tau I)V$ for some $V \in \mathbb{R}^{n\times k}$ (obtained in the Jacobi–Davidson method, e.g.):

$$V^H(A-\tau I)^HVz = \frac{1}{\theta-\tau}V^H(A-\tau I)^H(A-\tau I)Vz \qquad (*)$$

If $\frac{1}{\theta-\tau}$ is an extreme eigenvalue and z a corresponding eigenvector, then $(\frac{1}{\theta-\tau}, Wz)$ is an approximate eigenpair of $(A-\tau I)^{-1}$, and (θ, Wz) is an approximate eigenpair of A.

$Vz = (A-\tau I)^{-1}Wz$ generally is a better eigenvector approximation than Wz, because it is the result of applying one step of shifted inverse iteration to Wz with shift τ. Vz is called harmonic Ritz vector, and θ harmonic Ritz value.

The Rayleigh quotient ρ of Vz with respect to A often is a better approximation to an eigenvalue close to τ than θ.

Refined Ritz vectors

Given an approximate eigenvalue $\tilde\lambda$ (for instance a Ritz value θ or a target value τ) and a basis V of a search space $\mathcal{V}$. The refined Ritz vector is defined as

$$\tilde u = Vz \quad \text{where } z = \operatorname{argmin}_y \|(A-\tilde\lambda I)Vy\|.$$

Often, the refined Ritz vector $\tilde u$ is a much better approximation to an eigenvalue close to $\tilde\lambda$ than an ordinary Ritz vector.

Again, the Rayleigh quotient of $\tilde u$ often is a better approximate eigenvalue than $\tilde\lambda$.

Computing the refined Ritz vector is expensive (if $\mathcal{V}$ is not a Krylov space), because it requires the singular value decomposition of an $n\times k$ matrix at an additional cost of $\mathcal{O}(nk^2)$ flops at iteration k.

Moreover, since θ changes from one iteration to the next, we can not update the SVD from the previous iteration, and we have to compute a new SVD in each iteration.

Solving the correction equation

The correction equation

$$(I-u^k(u^k)^H)(A-\theta I)(I-u^k(u^k)^H)t = -(A-\theta I)u^k, \quad t\perp u^k$$

is solved iteratively by a preconditioned Krylov solver.

Suppose that K is a preconditioner for $A-\theta I$, i.e.

$$K^{-1}(A-\theta I) \approx I.$$

Since the eigenvalue approximation θ varies in the course of the algorithm the preconditioner should be altered as well. However, frequently K can be kept fixed for several iterations (and sometimes even when computing several eigenvalues).

When solving the correction equation one has to consider the restriction to the orthogonal complement of the current approximation u^k. This suggests to consider for fixed K with $K^{-1}(A-\theta I)\approx I$ the preconditioner

$$\tilde K := (I-u^k(u^k)^H)K(I-u^k(u^k)^H).$$

Solving the correction equation ct.

Consider a Krylov subspace solver for the correction equation with initial vector $t_0 = 0$ and left preconditioning.

Since the initial vector and u^k are orthogonal the orthogonality is maintained for all iterates. Hence, in every step we have to determine a vector $z := \tilde K^{-1}\tilde A w$ where

$$\tilde A := (I-u^k(u^k)^H)(A-\theta_k I)(I-u^k(u^k)^H).$$

Firstly, it follows from $(u^k)^Hw = 0$

$$\begin{aligned}\tilde Aw &= (I-u^k(u^k)^H)(A-\theta_k I)(I-u^k(u^k)^H)w\\ &= (I-u^k(u^k)^H)y\end{aligned}$$

with $y = (A-\theta_k I)w$.

Solving the correction equation ct.

With this notation we have to solve

$$\tilde{K}z = (I - u^k(u^k)^H)y.$$

From $z \perp u^k$ we obtain that z has to satisfy

$$Kz = y - \alpha u^k \quad \text{i.e.} \quad z = K^{-1}y - \alpha K^{-1}u^k,$$

and the requirement $z \perp u^k$ yields

$$\alpha = \frac{(u^k)^H K^{-1} y}{(u^k)^H K^{-1} u^k}.$$

Hence, in every step of the preconditioned Krylov method we have solve the linear system $K\tilde{y} = y$, and additionally at the beginning we have to solve the system $K\tilde{u} = u^k$.

Solving the correction equation ct.

The approximate solution of the correction equation by a preconditioned Krylov solver has the following form:

- solve $K\tilde{u} = u$ for $\tilde{u}$, and compute $\mu = u^H\tilde{u}$.
- determine $\tilde{r}$ from
  - (i) solve $K\hat{r} = \tilde{r}$ for $\hat{r}$
  - (ii) set $\tilde{r} = \hat{r} - \frac{u^H\hat{r}}{\mu}\hat{u}$
- Apply Krylov solver with initial vector $t_0 = 0$, matrix $\tilde{K}^{-1}\tilde{A}$ and right hand side $-\tilde{r}$. In each step determine $z = \tilde{K}^{-1}\tilde{A}w$ according to
  - (a) $y = (A - \theta I)w$.
  - (b) solve $K\hat{y} = y$ for $\hat{y}$
  - (c) $z = \hat{y} - \frac{u^H\hat{y}}{\mu}\hat{u}$

Jacobi-Davidson method; largest eigenvalue

1: Choose initial vector t, and set $U = []$, $V = []$
2: **for** $m = 1, 2, \ldots$ **do**
3: $t = t - UU^Ht$
4: $u = t/\|t\|$; $U = [U\ u]$; $v = Au$; $V = [V\ v]$
5: $C(1:m-1, m) = U(:, 1:m-1)^H V(:, m)$
6: $C(m, 1:m-1) = U(:, m)^H V(:, 1:m-1)$
7: $C(m, m) = U(:, m)^H V(:, m)$
8: Compute largest eigenvalue θ of C in modulus
and corresponding eigenvector s such that $\|s\| = 1$
9: $y = Us$
10: $r = Ay - \theta y$
11: **if** $\|r\| \le \varepsilon$ **then**
12: $\lambda = \theta$, $x = y$, STOP
13: **end if**
14: Solve approximately
$(I - yy^H)(A - \theta I)(I - yy^H)t = -r, \quad t \perp y$ for t
15: **end for**

Comments

In step 3. the classical Gram–Schmidt method for orthogonalizing t against U can be replaced by the modified Gram–Schmidt method. Observe, however, that the classical method takes advantage of BLAS level-3-operations, whereas the modified method uses only level-1-operations.

It is reasonable to repeat the orthogonalization, if $\|t - UU^Ht\|/\|t\|$ is small, i.e. if the angle between t and span$U$ is small. To this end we choose κ (which is not too small), for instance $\kappa = 0.25$, and replace step 3. by

1: $\tau = \|t\|$
2: $t = t - UU^Ht$
3: **if** $\|t\|/\tau \le \kappa$ **then**
4: $t = t - UU^Ht$
5: **end if**

Again (in both appearances) we can replace the classical by the modified Gram–Schmidt method.

Comments ct.

If A is Hermitean, then step 7. can be replaced by

$$C(m, 1:m-1) = C(1:m-1, m)^H$$

and the cost for updating the projection of A is cut by half approximately.

10. can be replaced by

$$r = Vs,$$

if m is smaller than the average filling of the rows of A

It is not necessary to solve the correction equation in 14. very accurately. Sleijpen and van der Vorst suggest a relative accuracy of 2^{-m} in the m-th step following the recommendation for the inexact Newton method. Notice that if the correction equation is solved exactly the Jacobi–Davidson method is a generalization of inverse iteration, which can be interpreted as Newton's method.

Comments ct.

As for the Arnoldi method the increasing storage and the computational overhead for increasing the dimension of the ansatz space may make it necessary to restart.

An obvious way is to restart with the most recent approximation to an eigenvector as initial vector. However, this destroys valuable information contained in the discarded part of the ansatz space, and the speed of convergence will be slowed down.

Therefore it is often a better strategy to restart with a subspace spanned by a small number of Ritz vectors or harmonic Ritz vectors corresponding to approximations close to the wanted eigenvalue (thick restart).

Notice that iterative projection methods which do not use Krylov subspaces are more flexible. Especially at restart, they can retain any number of approximate eigenvectors without the need of the implicit restarting framework.

Several eigenpairs

Quite often one is interested not only in one but in several eigenpairs.

The Jacobi–Davidson method often converges very rapidly to an eigenvalue (here the largest one), and the convergence often is faster than for Arnoldi's method. On the other hand Arnoldi yields approximations to several eigenvectors simultaneously whereas Jacobi-Davidson deliberately aims at one particular eigenvalue closest to some target.

Way out: Render converged eigenvectors harmless by deflation

Deflation

After an eigenvector has converged we continue with subspaces spanned by the remaining eigenvectors.

For Hermitean matrices this is no problem since the eigenvectors are orthogonal. In the correction equation one has to supplement the current Ritz vector by the already converged eigenvectors in the projector to the orthogonal complement.

For non-Hermitean matrices one works with Schur vectors.

Deflation ct.

If $u^1, \ldots, u^k$ denotes an orthonormal basis of the current search space and $C = U_k^H A U_k$, then we compute the Schur factorization $CV = VS$ of C, where V is an orthonormal matrix, and S is an upper triangular matrix (for instance by the QR algorithm for dense matrices).

Next we reorder S such that $|s_{ii} - \tau|$ is nonincreasing for some target value τ. This reordering can be done while preserving the upper triangular structure of S.

The first diagonal elements of S then represent eigenvalue approximations closest to τ, and the corresponding columns of $U_k V$ span an approximation to the invariant subspace of A corresponding to these eigenvectors.

The decomposition $A(U_k V) = (U_k V)S$ can be used in a restart, if one discards the columns of S and $U_k V$ corresponding to unwanted s_{ii}.

Deflation ct.

Assume that a partial Schur form $AU_k = U_k R_k$ is known which we want to complement by a new column u such that

$$A[U_k\ u] = [U_k\ u] \begin{bmatrix} R_k & s \\ & \lambda \end{bmatrix}, \quad U_k^H u = 0.$$

i.e.

$$\begin{aligned} AU_k &= U_k R_k \\ Au &= U_k s + \lambda u, \quad U_k^H u = 0. \end{aligned}$$

Multiplying the second equation by U_k^H yields

$$U_k^H A u = U_k^H U_k s + \lambda U_k^H u = s,$$

Deflation ct.

and substituting in the second equation one gets

$$Au = U_k U_k^H A u + \lambda u,$$

i.e.

$$(A - \lambda I)u = U_k U_k^H A u.$$

From $(A - \lambda I)U_k U_k^H u = 0$ it follows

$$(A - \lambda I)(I - U_k U_k^H)u = U_k U_k^H A u,$$

from which we obtain

$$(I - U_k U_k^H)(A - \lambda I)(I - U_k U_k^H)u = 0.$$

Deflation ct.

The last equation demonstrates that the new pair (u, λ) is an eigenpair of

$$\tilde{A} := (I - U_k U_k^H)A(I - U_k U_k^H)$$

which can be determined by the Jacobi–Davidson method.

To determine the next Schur vector u_{k+1} by the Jacobi–Davidson method one has to solve the correction equation

$$P_{k+1}(I - U_k U_k^H)(A - \theta I)(I - U_k U_k^H)P_{k+1}t = -r$$

where $P_{k+1} = I - uu^H$ and (θ, u) is the current Ritz pair.

Fokkema, Sleijpen, van der Vorst (1998) contains an example that demonstrates that the explicit deflation has to be used in the correction equation, but in the projection of A to the search space of the Jacobi–Davidson method the column vectors of U_k do not have to be taken account of.

Preconditioning

Preconditioning for an iterative solver for the correction equation considering explicit deflation is insignificantly more expensive than for the determination of the largest eigenvalue.

Let K be a preconditioner of $A - \theta I$, let (θ, u) be the current Ritz pair, and $\tilde{U} = [U_k, u]$.

The preconditioner K has to be restricted to the orthogonal complement of $\tilde{U}$, i.e. actually one has to precondition by

$$\tilde{K} = (I - UU^H)K(I - UU^H).$$

This can be done in a similar way as for $\tilde{U} = u$.

Preconditioning ct.

As for the largest eigenvalue it holds: If we apply a Krylov solver with initial vector $t_0 = 0$ with left preconditioning, then all iterates are contained in the orthogonal complement of $\tilde{U}$.

For a given vector v we have to find $z := \tilde{K}^{-1}\tilde{A}v$ in this space where

$$\tilde{A} := (I - \tilde{U}\tilde{U}^H)(A - \theta I)(I - \tilde{U}\tilde{U}^H).$$

Again this is done in two steps: First determine

$$\begin{aligned} \tilde{A}v &= (I - \tilde{U}\tilde{U}^H)(A - \theta I)(I - \tilde{U}\tilde{U}^H)v \\ &= (I - \tilde{U}\tilde{U}^H)y \end{aligned}$$

with $y := (A - \theta I)v$ (remember $\tilde{U}^H v = 0$).

Preconditioning ct.

Next we have to determine $z \perp \tilde{U}$ such that

$$\tilde{K}z = (I - \tilde{U}\tilde{U}^H)y,$$

i.e. on account of $\tilde{U}^H z = 0$

$$(I - \tilde{U}\tilde{U}^H)K(I - \tilde{U}\tilde{U}^H)z = (I - \tilde{U}\tilde{U}^H)Kz = (I - \tilde{U}\tilde{U}^H)y,$$

and hence

$$(I - \tilde{U}\tilde{U}^H)(Kz - y) = 0.$$

Therefore z satisfies

$$Kz = y - \tilde{U}\alpha \quad \text{i.e.} \quad z = K^{-1}y - K^{-1}\tilde{U}\alpha,$$

and the condition $\tilde{U}^H z = 0$ yields

$$\alpha = (\tilde{U}^H K^{-1}\tilde{U})^{-1}\tilde{U}K^{-1}y.$$

Preconditioning ct.

In each step of the preconditioned Krylov solver one needs the vector $\hat{y} = K^{-1}y$ and the matrix $\hat{U} = K^{-1}\tilde{U}$.

As before $\hat{U}$ is identical in all iteration steps. Therefore, to perform m iteration steps when solving the correction equation one has to solve $m + k + 1$ linear systems with system matrix K.

If the preconditioner is kept fixed while computing several eigenvalues then $\hat{U}$ can be reused for all of these eigenvalues.

Implementations of this algorithm in Fortran 77 and in MATLAB can be downloaded from the Homepage of Gerard Sleijpen.

Generalized Hermitean eigenproblems

Consider the generalized eigenvalue problem

$$Ax = \lambda Bx, \quad \text{where } A = A^H,\ B = B^H,\ B \text{ positive definite.}$$

Given an approximation (θ, x) to an eigenpair the inverse iteration is defined by $v := (A - \theta B)^{-1} Bx$. We expand the current search space by $t := x + \alpha v$, where α is chosen such that x and $x + \alpha v$ are orthogonal.

Measuring angles with respect to the scalar product $\langle x, y\rangle_B := x^H By$, then the robustness requirement $\langle x, x + \alpha v\rangle_B = 0$ yields the expansion

$$t = x - \frac{x^H Bx}{x^H B(A - \theta B)^{-1} Bx}(A - \theta B)^{-1} Bx,$$

which is the solution of the symmetric correction equation

$$\Big(I - \frac{Bxx^H}{x^H Bx}\Big)\Big(A - \theta B\Big)\Big(I - \frac{xx^H B}{x^H Bx}\Big)t = (A - \theta B)x, \quad t \perp_B x.$$

This is the correction equation introduced by Sleijpen, Booten, Fokkema & van der Vorst (1996) in a different way.

Generalized Hermitean eigenproblems ct.

The operator

$$\Big(I - \frac{Bxx^H}{x^H Bx}\Big)\Big(A - \theta B\Big)\Big(I - \frac{xx^H B}{x^H Bx}\Big)$$

maps the space $(Bx)^\perp$ onto the space $x^\perp$, so that preconditioning is always required if we use a Krylov solver in order to get a mapping of $(Bx)^\perp$ into itself.

Choosing

$$\tilde{K} = \Big(I - \frac{Bxx^H}{x^H Bx}\Big)K\Big(I - \frac{xx^H B}{x^H Bx}\Big)$$

with $K^{-1}(A - \theta B) \approx I$, the preconditioner can be implemented in a similar way as for the standard eigenproblem.

In particular, taking into account the projector when solving the correction equation with a preconditioned Krylov solver requires only one additional solve with the preconditioner K.

Generalized Hermitean eigenproblems ct.

As for the standard eigenvalue problem the Jacobi-Davidson method can be combined with restart and deflation.

If we want to work with orthogonal operators in the deflation, then we have to work with B-orthogonal matrices that reduce the given generalized system to (truncated) Schur form

$$AQ_k = Z_k D_k$$

where $Z_k = BQ_k$ and Q_k has B-orthogonal columns.

D_k is diagonal with k computed eigenvalues on its diagonal, and the columns of Q_k are eigenvectors of the pencil $A - \lambda B$.

This leads to the projection for the deflation with the first k eigenvectors

$$(I - Z_k Q_k^H)(A - \lambda B)(I - Q_k Z_k^H).$$

It is easy to verify that the deflated operator B is still symmetric and positive definite with respect to the space $(BQ_k)^\perp$.

Generalized eigenproblems

Consider the generalized eigenvalue problem

$$Ax = \lambda Bx$$

with general matrices $A, B \in \mathbb{C}^{n\times n}$ and B is nonsingular.
Then given an approximation (θ, x) to an eigenpair the inverse iteration is defined by $v := (A - \theta B)^{-1} Bx$.

Expanding the current search space by $t := x + \alpha v$, where α is chosen such that x and $x + \alpha v$ are orthogonal with respect to the Euclidean inner product, we obtain

$$t = x - \frac{x^H x}{x^H (A - \theta B)^{-1} Bx}(A - \theta B)^{-1} Bx.$$

t this is the solution of the well known correction equation

$$\Big(I - \frac{Bxx^H}{x^H Bx}\Big)\Big(A - \theta B\Big)\Big(I - \frac{xx^H}{x^H x}\Big)t = (A - \theta B)x, \quad t \perp x$$

of the Jacobi–Davidson method; cf. Fokkema, Sleijpen & van der Vorst (1998).

Two-sided Jacobi-Davidson

We already mentioned that the Jacobi-Davidson method can be considered as an acceleration of inverse iteration with Rayleigh quotient shifts (Rayleigh quotient iteration).

$$\tilde{u}^{k+1} = (A - \theta_k I)^{-1} u^k, \; u^{k+1} = \frac{\tilde{u}^{k+1}}{\|\tilde{u}^{k+1}\|}, \; \theta_{k+1} = (u^{k+1})^T A u^{k+1}.$$

The Rayleigh quotient iteration (RQI) is known to converge cubically to simple eigenvalues of normal matrices. For a (nonnormal) eigenvalue of a nonnormal matrix it converges locally quadratic at best (cf. Parlett 1974).

Ostrowski's two sided RQI works with the two-sided (or generalized) Rayleigh quotient

$$\theta(u, v) := \frac{v^H A u}{v^H u}$$

where u and v are approximate left and right eigenvectors, respectively.

In Parlett (1975) it was shown that the two-sided RQI converges locally and cubically to simple eigenvalues.

Two-sided Rayleigh quotient iteration

1: Choose initial vector u^1 and v^1 with unit norm such that $(v^1)^H u^1 \neq 0$
2: **for** $k = 1, 2, \ldots$ **do**
3: compute $\theta_k = \frac{(v^k)^H A u^k}{(v^k)^H u^k}$
4: **if** $A - \theta_k I$ sufficiently singular **then**
5: solve $(A - \theta_k I)x = 0$ and $(A^H - \overline{\theta_k} I)y = 0$
6: STOP
7: **end if**
8: solve $(A - \theta_k I)u^{k+1} = u^k$ and normalize u^{k+1}
9: solve $(A^H - \overline{\theta_k} I)v^{k+1} = v^k$ and normalize v^{k+1}
10: **if** $(v^{k+1})^H u^{k+1} = 0$ **then**
11: the method fails
12: **end if**
13: **end for**

Two-sided Jacobi-Davidson

The two-sided RQI suggests to work with two search spaces $\mathcal{U}$ for the right eigenvector, and $\mathcal{V}$ for the left eigenvector.

Suppose that we have k dimensional search spaces $\mathcal{U}$ and $\mathcal{V}$, and approximations $u \in \mathcal{U}$ and $v \in \mathcal{V}$ to right and left eigenvectors where $v^H u \neq 0$. Then we choose the Rayleigh quotient

$$\theta = \theta(u, v) := \frac{v^H A u}{v^H u} \qquad (1)$$

as approximation to the corresponding eigenvalue.

Note that (1) hold if and only if

$$Au - \theta u \perp v \quad \text{and} \quad A^H v - \overline{\theta} v \perp u.$$

$u = Uc$ and $v = Vd$ (where the columns of U and V form an orthonormal basis of $\mathcal{U}$ and $\mathcal{V}$, respectively) are chosen as eigenvectors of the oblique projection of A to $\mathcal{U}$ along $\mathcal{V}$, i.e.

$$V^H A U c = \theta V^H U c \quad \text{and} \quad U^H A V d = \overline{\theta} U^H V d.$$

Two-sided Jacobi-Davidson ct.

Similar to the original Jacobi-Davidson method we expand the search spaces such that the directions of inverse iteration are contained in the augmented spaces:

$$s = u + \alpha(A - \theta I)^{-1} u \quad \text{and} \quad t = v + \beta(A^H - \overline{\theta} I)^{-1} v.$$

For robustness reasons we choose α such that $s \perp u$ and $t \perp v$, i.e.

$$\alpha = -\frac{\|u\|^2}{u^H (A - \theta I)^{-1} u} \quad \text{and} \quad \beta = -\frac{\|v\|^2}{v^H (A^H - \overline{\theta} I)^{-1} v}.$$

Hence, s is a solution of a projected problem

$$\left(I - \frac{u p^H}{p^H u}\right)(A - \theta I)(I - u u^H) s = (A - \theta I) u, \quad s \perp u,$$

for some $p \in \mathbb{C}^n$, and for consistency reasons we choose $p = v$, since by construction $(A - \theta I)u \in v^\perp$.
Similarly the correction equation for t reads

$$\left(I - \frac{v u^H}{u^H v}\right)(A^H - \overline{\theta} I)(I - v v^H) t = (A^H - \overline{\theta} I) v, \quad t \perp v,$$

Two-sided Jacobi-Davidson algorithm

1: Choose initial vector u^1 and v^1 with unit norm such that $(v^1)^H u^1 \neq 0$
2: $s = u^1$; $t = v^1$; $U_0 = []$; $V_0 = []$
3: **for** $k = 1, 2, \ldots$ **do**
4: $U_k = MGS(U_{k-1}, s)$; $V_k = MGS(V_{k-1}, t)$
5: compute kth column of $W_k = AU_k$
6: compute kth row and column of $H_k = V_k^H W_k$
7: compute wanted eigentripel (θ, c, d) of the pencil $(V_k^H A U_k, V_k^H U_k)$
8: $u = U_k c$; $v = V_k d$;
9: $r_u = (A - \theta I)u = W_k c - \theta u$;
10: $r_v = (A^H - \overline{\theta} I)v$
11: STOP if $\min\{\|r_u\|, \|r_v\|\} \leq$ tol
12: Solve (approximately) $s \perp u$ and $t \perp v$ from

$$\Big(I - \frac{uv^H}{v^H u}\Big)(A - \theta I)(I - uu^H)s = (A - \theta I)u, \quad s \perp u$$

$$\Big(I - \frac{vu^H}{u^H v}\Big)(A^H - \overline{\theta} I)(I - vv^H)t = (A^H - \overline{\theta} I)v, \quad t \perp v,$$

13: **end for**

Remarks

Hochstenbach & Sleijpen (2003) proposed the two-sided Jacobi-Davidson method with a different motivation. They further suggested a further variant where the bases U_k and V_k are constructed to be bi-orthogonal.

Here, the expansions s and t of U_k and V_k satisfy the correction equations

$$\Big(I - \frac{uv^H}{v^H u}\Big)(A - \theta I)\Big(I - \frac{uv^H}{v^H u}\Big)s = (A - \theta I)u, \quad s \perp v$$

$$\Big(I - \frac{vu^H}{u^H v}\Big)(A^H - \overline{\theta} I)\Big(I - \frac{vu^H}{u^H v}\Big)t = (A^H - \overline{\theta} I)v, \quad t \perp u,$$

Schwetlick & Schreiber (2006) used arguments from bifurcation theory to motivate a variant of the Jacobi-Davidson method which is based on the correction equations

$$(I - vv^H)(A - \theta I)(I - uu^H)s = (A - \theta I)u, \quad s \perp u$$

$$(I - uu^H)(A^H - \overline{\theta} I)(I - vv^H)t = (A^H - \overline{\theta} I)v, \quad t \perp v$$

All 3 methods converge locally and cubically