Numerical Linear Algebra for Computational Science and Information Engineering

Jacobi-Davidson Methods

Nicolas Venkovic
nicolas.venkovic@tum.de

Chair of Computational Mathematics
School of Computation, Information and Technology
Technical University of Munich

Outline I

Motivation

- **Rayleigh-Ritz projections in Krylov subspaces** from Lanczos/Arnoldi procedures are very **effective to compute exterior eigenpairs**, provided the targeted eigenvalues are well-separated from the rest of the spectrum.
- In combination with a **shift-and-invert** spectral transformation, Rayleigh-Ritz projections in Krylov subspaces are also **efficient to compute interior eigenpairs** in the vicinity of a shift σ.

  A proper implementation of shift-and-invert transformations requires an evaluation of the mapping $x \mapsto (A - \sigma I_n)^{-1} x$ at each iteration.
- The **Jacobi-Davidson** method is of particular interest when one cannot afford to evaluate $x \mapsto (A - \sigma I_n)^{-1} x$ with sufficient precision.

  The Jacobi-Davidson method was proposed by Sleijpen and Van der Vorst (2000) on the basis of ideas from Jacobi (1845-46) and Davidson (1975).

Sleijpen, G. L., & Van der Vorst, H. A. (2000). A Jacobi–Davidson iteration method for linear eigenvalue problems. SIAM review, 42(2), 267-293.

Jacobi, C.G.J. (1845), Ueber eine neue Auflosungsart der bei der Methode der kleinsten Quadrate vorkommende linearen Gleichungen, Astronom Nachr, 297-306.

Jacobi, C. G. J. (1846). Über ein leichtes Verfahren die in der Theorie der Säcularstörungen vorkommenden Gleichungen numerisch aufzulösen. J. Reine Angew. Math., 30, 51–94.

Davidson E. R. (1975). The iterative calculation of a few of the lowest eigenvalues and corresponding eigenvectors of large real symmetric matrices. J. Comput. Phys., 17, 87–94.

Davidson method

Davidson method

- In the Davidson (1975) method, one is equipped with an **orthonormal basis** in the columns of $Q_k := [q_1, \ldots, q_k] \in \mathbb{F}^{n \times k}$.

  A **Rayleigh-Ritz projection** in range(Q_k) is deployed where range(Q_k) is ***not*** **a Krylov subspace**. We search for $(\lambda, \hat{y}) \in \mathbb{F} \times \mathbb{F}^k$ such that

$$B_k \hat{y} = \lambda \hat{y}$$

  where $B_k := Q_k^H A Q_k$. We then have a Rayleigh-Ritz pair (λ, y) in which $y := Q_k \hat{y}$, and a residual given by $r := Ay - \lambda y$.
- The purpose of the Davidson method is to **improve the Rayleigh-Ritz vector** y to decrease the residual norm $\|r\|_2$.

  For this, Davidson (1975) suggests to compute the **expansion vector** $t \in \mathbb{F}^n$ such that

$$(D_A - \lambda I_n) t = r$$

  where $D_A \in \mathbb{F}^{n \times n}$ is the diagonal matrix formed with the diagonal A.

Davidson E. R. (1975). The iterative calculation of a few of the lowest eigenvalues and corresponding eigenvectors of large real symmetric matrices. J. Comput. Phys., 17, 87–94.

Davidson method, cont'd$_1$

- The **expansion vector** t is then **orthogonalized** against $q_1, \ldots, q_k$, **normalized** and **used to expand the search space**:

Solve for t such that $(D_A - \lambda I_n)t = r$
$t := \Pi^{(k)} t$ $\quad$ $//\Pi^{(k)}$ is a projector onto range$(Q_k)^\perp$
$q_{k+1} := t/\|t\|_2$

  New Rayleigh-Ritz pairs can then be sought in range(Q_{k+1}).
- The Davidson method has shown great success to approximate **exterior eigenpairs** of **diagonally dominant**, *but not diagonal*, matrices A.
  Indeed, **if A is diagonal**, then

$$t = (D_A - \lambda I_n)^{-1} r = (A - \lambda I_n)^{-1}(A - \lambda I_n)y = y \in \text{range}(Q_k)$$

  so that **the search space range(Q_k) cannot be expanded with t.**
  Then the method **stagnates** and becomes unable to achieve convergence.
- If $D_A \propto I_n$, then the Davidson method is equivalent to Lanczos or Arnoldi.

Davidson E. R. (1975). The iterative calculation of a few of the lowest eigenvalues and corresponding eigenvectors of large real symmetric matrices. J. Comput. Phys., 17, 87–94.

Davidson method, cont'd$_2$

- Although the Davidson method was originaly applied to real symmetric matrices, it seamlessly applies to non-symmetric/Hermitian matrices.

  For **non-symmetric/Hermitian** matrices, the algorithm is as follows:

Algorithm 1 Davidson: $(A, q, k) \mapsto (\lambda, y)$

1: Allocate memory for $Q_k, W_k \in \mathbb{F}^{n\times k}$ and $B_k \in \mathbb{F}^{k\times k}$
2: $q_1 := q/\|q\|_2$
3: **for** $j = 1, \ldots, k$ **do**
4: $\quad w_j := Aq_j$
5: $\quad B_k[1:j, j] := Q_j^H w_j$, $B_k[j, 1:j-1] := q_j^H W_{j-1}$
6: $\quad$ Solve for an exterior eigenpair $(\lambda, \hat{y})$ of B_j $\quad \triangleright\ B_j := B_k[1:j, 1:j]$
7: $\quad y := Q_j \hat{y}$
8: $\quad r := Ay - \lambda y$
9: $\quad$ Solve for t such that $(D_A - \lambda I_n)t = r$
10: $\quad t := \Pi^{(j)} t$ $\quad \triangleright\ \Pi^{(j)}$ is a projector onto range$(Q_j)^\perp$
11: $\quad q_{j+1} := t/\|t\|_2$

Davidson E. R. (1975). The iterative calculation of a few of the lowest eigenvalues and corresponding eigenvectors of large real symmetric matrices. J. Comput. Phys., 17, 87–94.

Davidson method, cont'd$_3$

- For **Hermitian matrices**, the algorithm is as follows:

Algorithm 2 Davidson: $(A, q, k) \mapsto (\lambda, y)$

1: Allocate memory for $Q_k \in \mathbb{F}^{n \times k}$ and $B_k \in \mathbb{F}^{k \times k}$
2: $q_1 := q/\|q\|_2$
3: **for** $j = 1, \ldots, k$ **do**
4: $\quad w := Aq_j$
5: $\quad B_k[1:j, j] := Q_j^H w$ ▷ $B_k[j, 1:j-1] := B_k[1:j-1, j]^T$
6: $\quad$ Solve for an exterior eigenpair $(\lambda, \hat{y})$ of B_j ▷ $B_j := B_k[1:j, 1:j]$
7: $\quad y := Q_j \hat{y}$
8: $\quad r := Ay - \lambda y$
9: $\quad$ Solve for t such that $(D_A - \lambda I_n)t = r$
10: $\quad t := \Pi^{(j)} t$ ▷ $\Pi^{(j)}$ is a projector onto range$(Q_j)^\perp$
11: $\quad q_{j+1} := t/\|t\|_2$

Although $\Pi^{(j)}$ is most commonly defined as a MGS procedure, CGS2 can also be used to mitigate potential stagnation, see van der Vorst (2002).

Davidson E. R. (1975). The iterative calculation of a few of the lowest eigenvalues and corresponding eigenvectors of large real symmetric matrices. J. Comput. Phys., 17, 87–94.
van der Vorst, H. A. (2002). Computational methods for large eigenvalue problems.

Generalized Davidson (GD) method

Generalized Davidson method

- Some modificiations of the Davidson method introduced by Morgan & Scott (1986) as well as Crouzeix et al. (1994) lead to variants collectively referrred to as the **generalized Davidson (GD)** method.

  Morgan & Scott (1986):
  - A **general preconditioner** of the form $M - \vartheta I_n$ is used instead of the original $D_A - \lambda I_n$, **without requirement of positive-definiteness**.
  - The aim is for $M - \vartheta I_n$ to **approximate** $A - \lambda I_n$ while allowing for **fast evaluation of** $r \mapsto (M - \vartheta I_n)^{-1} r$.
  - The **preconditioner should not be too good** to avoid stagnation, i.e.,

$$M - \vartheta I_n = A - \lambda I_n \implies t := (M - \vartheta I_n)^{-1} r = y \in \text{range}(Q_k).$$

    This **contradicts the common notion of preconditioner**.
  - Numerical results reported with significantly **improved convergence** behaviors when **letting** M **be the tridiagonal form of** A and $\vartheta := \lambda$.
  - Upon setting $\vartheta := \sigma$, one can **drive global convergence** toward some σ.

Morgan, R. B., & Scott, D. S. (1986). Generalizations of Davidson's method for computing eigenvalues of sparse symmetric matrices. SIAM Journal on Scientific and Statistical Computing, 7(3), 817-825.

Generalized Davidson method, cont'd$_1$

Morgan (1991):

- **Harmonic Ritz** pairs are used to yield even **faster convergence towards interior eigeinpairs**.

Crouzeix et al. (1994):

- **Several eigenpairs** are sought **at the same time** and **several vectors** are **incorporated into each search space expansion**, leading to a **block implementation**.
- A **maximum search space dimension** is introduced, triggering periodic **restarts** of the iterative method.
- **Restarting** of the GD method **renders convergence dependent on positive-definiteness of the preconditioners**.

Sadkane (1993):

- **Extension** of the GD method **to real non-symmetric matrices**.

Morgan, R. B. (1991). Computing interior eigenvalues of large matrices. Linear Algebra and its Applications, 154, 289-309.

Crouzeix, M., Philippe, B., & Sadkane, M. (1994). The Davidson method. SIAM Journal on Scientific Computing, 15(1), 62-76.

Sadkane, M. (1993). Block-Arnoldi and Davidson methods for unsymmetric large eigenvalue problems. Numerische Mathematik, 64, 195-211.

Generalized Davidson method, cont'd$_2$

- The computation of Rayleigh-Ritz pairs after the generalized Davidson (GD) method is as follows:

Algorithm 3 GD: $(A, q, k) \mapsto (\lambda, y)$

1: Allocate memory for $Q_k, W_k \in \mathbb{F}^{n\times k}$ and $B_k \in \mathbb{F}^{k\times k}$
2: $q_1 := q/\|q\|_2$
3: **for** $j = 1, \ldots, k$ **do**
4: $\quad w_j := Aq_j$
5: $\quad B_k[1:j, j] := Q_j^H w_j$, $B_k[j, 1:j-1] := q_j^H W_{j-1}$
6: $\quad$ Solve for an exterior eigenpair $(\lambda, \hat{y})$ of B_j $\quad \triangleright\ B_j := B_k[1:j, 1:j]$
7: $\quad y := Q_j \hat{y}$
8: $\quad r := Ay - \lambda y$
9: $\quad$ Solve for t such that $(M - \lambda I_n)t = r$
10: $\quad t := \Pi^{(j)} t$ $\quad \triangleright\ \Pi^{(j)}$ is a projector onto range$(Q_j)^\perp$
11: $\quad q_{j+1} := t/\|t\|_2$

Generalized Davidson method, cont'd$_3$

- For a **harmonic Ritz** pair (λ, y) with respect to a search space range(Q_k), there exists $\hat{y} \in \mathbb{F}^k$ such that $y = Q_k \hat{y}$ and

$$G_1 \hat{y} = \lambda G_2^H \hat{y}$$

where $G_1 := ((A - \sigma I_n)Q_k)^H (A - \sigma I_n)Q_k$ and $G_2 := Q_k^H (A - \sigma I_n)Q_k$. If A is non-Hermitian, a **basic implementation** of the harmonic GD method is as follows:

Algorithm 4 Basic harmonic GD: $(A, q, \sigma, k) \mapsto (\lambda, y)$

1: Allocate memory for $Q_k, W_k \in \mathbb{F}^{n \times k}$ and $G_1, G_2 \in \mathbb{F}^{k \times k}$
2: $q_1 := q/\|q\|_2$
3: **for** $j = 1, \ldots, k$ **do**
4: $\quad w_j := (A - \sigma I_n) q_j$
5: $\quad G_1[1:j, j] := W_j^H w_j$ ▷ $G_1[j, 1:j-1] := G_1[1:j-1, j]^H$
6: $\quad G_2[1:j, j] := Q_j^H w_j$, $G_2 := [j, 1:j-1] := q_j^H W_{j-1}$
7: $\quad$ Solve for eigenpair $(\lambda, \hat{y})$ of $G_2[1:j, 1:j]^{-H} G_1[1:j, 1:j]$ closest to 0
8: $\quad y := Q_j \hat{y}$, $\delta_\rho := \hat{y}^H G_2 \hat{y}$, $\rho := \sigma + \delta_\rho$, $r := W_j \hat{y} - \delta_\rho y$
9: $\quad$ Solve for t such that $(M - \rho I_n)t = r$
10: $\quad t := \Pi^{(j)} t$, $q_{j+1} := t/\|t\|_2$ ▷ $\Pi^{(j)}$ is a projector onto range$(Q_j)^\perp$

Jacobi methods

Orthogonal complement corrections

- **Jacobi orthogonal complement correction (JOCC)**:
  Jacobi (1845) considered an eigenvalue problem as a linear system of equations for which an iterative solver, e.g., Jacobi iteration, is used as a means to generate a **sequence of orthogonal complement corrections to a given approximate eigenvector**.
  - Suppose we have a **strongly diagonally dominant** matrix A, of which $\alpha := a_{11}$ is the largest element.
  - Then (α, e_1) is an **approximation** of the **largest eigenpair** (θ, z) of A.
  - In matrix notation, the JOCC approach is as follows. Consider

$$A\left(e_1 + \begin{bmatrix} 0 \\ w \end{bmatrix}\right) = \theta\left(e_1 + \begin{bmatrix} 0 \\ w \end{bmatrix}\right)$$

$$\begin{bmatrix} \alpha & c^T \\ b & F \end{bmatrix}\left(e_1 + \begin{bmatrix} 0 \\ w \end{bmatrix}\right) = \theta\left(e_1 + \begin{bmatrix} 0 \\ w \end{bmatrix}\right)$$

  where $[0\, w^T]^T$ is an **orthogonal complement correction** to the approximate eigenvector e_1.

Jacobi, C.G.J. (1845), Ueber eine neue Auflosungsart der bei der Methode der kleinsten Quadrate vorkommende linearen Gleichungen, Astronom Nachr, 297-306.

Orthogonal complement corrections, cont'd

- The eigenvalue problem leads to the following equations:

$$\lambda = \alpha + c^T w$$
$$(F - \lambda I_n)w = -b$$

  which Jacobi proceeded to solve with the following iteration:

$$\lambda_k := \alpha + c^T w_k$$
$$(D_F - \lambda_k I_n)w_{k+1} = (D_F - F)w_k - b$$

  with $w_1 := 0$.
- This later became known as the **Jacobi iteration**.
- Although λ_k is not a Rayleigh-Ritz value, it is nevertheless an approximation of the largest eigenvalue θ.

- As the **JOCC** approach is **best-suited for strongly diagonally dominant matrices**, Jacobi (1846) coupled this approach with a **set of rotations** whose application **makes the matrix more diagonally dominant**.

Jacobi, C.G.J. (1845), Ueber eine neue Auflosungsart der bei der Methode der kleinsten Quadrate vorkommende linearen Gleichungen, Astronom Nachr, 297-306.

Jacobi, C. G. J. (1846). Über ein leichtes Verfahren die in der Theorie der Säcularstörungen vorkommenden Gleichungen numerisch aufzulösen. J. Reine Angew. Math., 30, 51–94.

Jacobi-Davidson method

JOCC by Sleijpen and van der Vorst (1996)

- Sleijpen and van der Vorst (2000) revisited the JOCC approach in the more general setting where an arbitrary iterate $y_j \in \mathbb{F}^n$ is known as an approximate eigenvector of $A \in \mathbb{F}^{n \times n}$.

  JOCC's adaptation to this more general context lies in setting a correction $\delta \in \mathbb{F}^n$ to y_j with unit norm such that

$$A(y_j + \delta) = \theta(y_j + \delta), \quad \delta \perp y_j \tag{1}$$

  where θ is the wanted eigenvalue of A.

  Eq. (1) can be decomposed into two parts, along and orthogonal to y_j:

  - First, the **part parallel to** y_j, given by

$$y_j y_j^H A(y_j + \delta) = \theta y_j y_j^H (y_j + \delta)$$

    is such that $\boxed{\vartheta_j + y_j^H A\delta = \theta}$ where $\boxed{\vartheta_j := y_j^H A y_j}$ is the **corrected eigenvalue estimate**.

Sleijpen, G. L., & Van der Vorst, H. A. (2000). A Jacobi–Davidson iteration method for linear eigenvalue problems. SIAM review, 42(2), 267-293.

JOCC by Sleijpen and van der Vorst (1996), cont'd

- Second, the **part orthogonal to** y_j, given by

$$(I_n - y_j y_j^H)A(y_j + \delta) = \theta(I_n - y_j y_j^H)(y_j + \delta)$$

is such that $(I_n - y_j y_j^H)(A - \theta I_n)\delta = (I_n - y_j y_j^H)(-Ay_j + \theta y_j)$

$$= -(I_n - y_j y_j^H)Ay_j$$

$$= -(Ay_j - \vartheta_j y_j) =: -r_j.$$

Since $\delta \perp y_j$, we have $\delta = (I_n - y_j y_j^H)\delta$, and we obtain:

$$(I_n - y_j y_j^H)(A - \theta I_n)(I_n - y_j y_j^H)\delta = -r_j$$

where θ, which **is unknown**, is replaced by ϑ_j to yield the **Jacobi-Davidson correction equation** given by:

$$\boxed{(I_n - y_j y_j^H)(A - \vartheta_j I_n)(I_n - y_j y_j^H)\delta = -r_j}.$$

Note that $r_j^H y_j = y_j^H A y_j - \vartheta_j = 0 \implies r_j \perp y_j$ so that **this equation is consistent as long as** $A - \vartheta_j I_n$ **is not singular**.

Sleijpen, G. L., & Van der Vorst, H. A. (1996). A Jacobi–Davidson iteration method for linear eigenvalue problems. SIAM review, 42(2), 267-293.

Exact solution of the Jacobi-Davidson correction equation

- The Jacobi-Davidson correction equation is such that

$$(I_n - y_j y_j^H)(A - \vartheta_j I_n)\delta = -r_j, \quad \delta \perp y_j$$
$$(A - \vartheta_j I_n)\delta - y_j y_j^H (A - \vartheta_j I_n)\delta = -r_j$$

so that $(A - \vartheta_j I_n)\delta = \alpha y_j - r_j$ where $\alpha := y_j^H (A - \vartheta_j I_n)\delta$. If ϑ_j is not an exact eigenvalue of A, then we get

$$\delta = \alpha (A - \vartheta_j I_n)^{-1} y_j - (A - \vartheta_j I_n)^{-1} r_j.$$

And from the orthogonality condition $y_j \perp \delta$, we get

$$\alpha = \frac{y_j^H (A - \vartheta_j I_n)^{-1} r_j}{y_j^H (A - \vartheta_j I_n)^{-1} y_j}.$$

Then, we set:

$$\begin{aligned} y_{j+1} &:= y_j + \delta \\ &= y_j + \alpha (A - \vartheta_j I_n)^{-1} y_j - (A - \vartheta_j I_n)^{-1} r_j \\ &= \alpha (A - \vartheta_j I_n)^{-1} y_j \end{aligned}$$

which corresponds to a **Rayleigh quotient iteration**.

Iterative solve of the Jacobi-Davidson equation

- In practice, the **J-D correction equation** is only **solved approximately**, typically using either MINRES (Paige & Saunders, 1975) when A is symmetric/Hermitian, or GMRES (Saad & Schultz, 1986) or even BiCGSTAB (Van der Vorst, 1992), when A is non-Hermitian.
- **At every step** j of the iteration, one has to **solve a linear system with a varying shift**.
- Based on the decomposition of the orthogonal correction δ presented by Sleijpen and van der Vorst (2000), a preconditioning of the following form is proposed:

$$r \mapsto \alpha M^{-1} y_j + M^{-1} r \text{ where } \alpha := \frac{y_j^H M^{-1} r}{y_j^H M^{-1} y_j},$$

in which M serves as an approximation of $A - \vartheta_j I_n$.

Paige, C.C. & M.A. Saunder (1975). Solution of sparse indefinite systems of linear equations. SIAM, J Numer Anal 12, 617-629.
Saad, Y. & Schultz M.H. (1986). GMRES: a generalized minimal residual algorithm for solving nonsymmetric linear systems, SIAM J Sci Statist Comput 7, 856-869.
van der Vorst, H. A. (1992). Bi-CGSTAB: A fast and smoothly converging variant of Bi-CG for the solution of nonsymmetric linear systems. SIAM Journal on scientific and Statistical Computing, 13(2):631–644.
Sleijpen, G. L. G. & van der Vorst, H. A. (2000). A Jacobi–Davidson iteration method for linear eigenvalue problems, SIAM Review, 42(2), 267–293.

Jacobi-Davidson algorithm with Rayleigh-Ritz projections

- Applying the Jacobi-Davidson (J-D) method to Rayleigh-Ritz projections, we obtain the following algorithm:

Algorithm 5 J-D: $(A, q, k) \mapsto (\lambda, y)$

1: Allocate memory for $Q_k, W_k \in \mathbb{F}^{n\times k}$ and $B_k \in \mathbb{F}^{k\times k}$
2: $\tilde{t} := q$
3: **for** $j = 1, \ldots, k$ **do**
4: $\quad \tilde{t} := \Pi^{(j-1)}\tilde{t}$ ▷ $\Pi^{(j)}$ is a projector onto range$(Q_j)^{\perp}$
5: $\quad q_j := \tilde{t}/\|\tilde{t}\|_2$
6: $\quad w_j := Aq_j$
7: $\quad B_k[1:j, j] := Q_j^H w_j,\ B_k[j, 1:j-1] := q_j^H W_{j-1}$
8: $\quad$ Solve for eigenpair $(\lambda, \hat{y})$ of B_j
9: $\quad y := Q_j \hat{y}$
10: $\quad r := W_j \hat{y}_j - \lambda y$
11: $\quad$ Solve for $\tilde{t} \approx t$ such that $(I_n - y_j y_j^H)(A - \lambda I_n)(I_n - y_j y_j^H)t = r$

Jacobi-Davidson algorithm with harmonic Ritz projections

- We saw in previous lectures that Rayleigh-Ritz projections converge first towards exterior eigenpairs, generally offering only poor approximations of interior pairs.
- Harmonic Ritz projections are the method of choice to find better approximations of interior eigenpairs.

Jacobi-Davidson algorithm with harmonic Ritz projections, cont'd

- Similarly as we previously saw for the GD method, the use of harmonic Ritz projections is recommended when trying to approximate interior eigenpair:

Algorithm 6 Basic harmonic J-D: $(A, q, \sigma, k) \mapsto (\lambda, y)$

1: Allocate memory for $Q_k, W_k \in \mathbb{F}^{n\times k}$ and $G_1, G_2 \in \mathbb{F}^{k\times k}$
2: $\tilde{t} := q$
3: **for** $j = 1, \ldots, k$ **do**
4: $\quad \tilde{t} := \Pi^{(j-1)}\tilde{t}$ ▷ $\Pi^{(j)}$ is a projector onto range$(Q_j)^{\perp}$
5: $\quad q_j := \tilde{t}/\|\tilde{t}\|_2$
6: $\quad w_j := (A - \sigma I_n)q_j$
7: $\quad G_1[1:j, j] := W_j^H w_j$ ▷ $G_1[j, 1:j-1] := G_1[1:j-1, j]^H$
8: $\quad G_2[1:j, j] := Q_j^H w_j$, $G_2[j, 1:j-1] := q_j^H W_{j-1}$
9: $\quad$ Solve for eigenpair $(\lambda, \hat{y})$ of $G_2[1\!:\!j, 1\!:\!j]^{-H} G_1[1\!:\!j, 1\!:\!j]$ closest to 0
10: $\quad y := Q_j \hat{y}$
11: $\quad \delta_\rho := \hat{y}^H G_2 \hat{y}$, $\rho := \sigma + \delta_\rho$
12: $\quad r := W_j \hat{y}_j - \delta_\rho y$