

# Numerical Linear Algebra for Computational Science and Information Engineering

## Lecture 12 Jacobi-Davidson method

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# 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  $\sigma$ .

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. (1996). A Jacobi–Davidson iteration method for linear eigenvalue problems. SIAM review, 42(2), 267-293.

Jacobi, C.G.J. (1845), Ueber eine neue Auflösungsart 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  $Q_k := [q_1, \dots, q_k] \in \mathbb{F}^{n \times k}$ .  
A **Rayleigh-Ritz projection** in  $\text{range}(Q_k)$  is deployed where  $\text{range}(Q_k)$  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  $(\lambda, y)$  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<sub>1</sub>

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

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

New Rayleigh-Ritz pairs can then be sought in  $\text{range}(Q_{k+1})$ .

- ▶ 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**  $\text{range}(Q_k)$  **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<sub>2</sub>

- Although the Davidson method was originally 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**  $j = 1, \dots, k$  **do**
  - 4:    $w_j := Aq_j$
  - 5:    $B_k[1 : j, j] := Q_j^H w_j, B_k[j, 1 : j - 1] := q_j^H W_{j-1}$
  - 6:   Solve for an exterior eigenpair  $(\lambda, \hat{y})$  of  $B_j$   $\triangleright B_j := B_k[1 : j, 1 : j]$
  - 7:    $y := Q_j \hat{y}$
  - 8:    $r := Ay - \lambda y$
  - 9:   Solve for  $t$  such that  $(D_A - \lambda I_n)t = r$
  - 10:    $t := \Pi^{(j)} t$   $\triangleright \Pi^{(j)}$  is a projector onto  $\text{range}(Q_j)^\perp$
  - 11:    $q_{j+1} := t / \|t\|_2$
- 

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<sub>3</sub>

► 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**  $j = 1, \dots, k$  **do**
  - 4:    $w := Aq_j$
  - 5:    $B_k[1 : j, j] := Q_j^H w$   $\triangleright B_k[j, 1 : j - 1] := B_k[1 : j - 1, j]^T$
  - 6:   Solve for an exterior eigenpair  $(\lambda, \hat{y})$  of  $B_j$   $\triangleright B_j := B_k[1 : j, 1 : j]$
  - 7:    $y := Q_j \hat{y}$
  - 8:    $r := Ay - \lambda y$
  - 9:   Solve for  $t$  such that  $(D_A - \lambda I_n)t = r$
  - 10:    $t := \Pi^{(j)} t$   $\triangleright \Pi^{(j)}$  is a projector onto  $\text{range}(Q_j)^\perp$
  - 11:    $q_{j+1} := t / \|t\|_2$
- 

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 modifications of the Davidson method introduced by Morgan & Scott (1986) as well as Crouzeix et al. (1994) lead to variants collectively referred 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  $\sigma$ .

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<sub>1</sub>

Morgan (1991):

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

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<sub>2</sub>

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

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

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- 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**  $j = 1, \dots, k$  **do**
  - 4:    $w_j := Aq_j$
  - 5:    $B_k[1 : j, j] := Q_j^H w_j, B_k[j, 1 : j - 1] := q_j^H W_{j-1}$
  - 6:   Solve for an exterior eigenpair  $(\lambda, \hat{y})$  of  $B_j$  ▷  $B_j := B_k[1 : j, 1 : j]$
  - 7:    $y := Q_j \hat{y}$
  - 8:    $r := Ay - \lambda y$
  - 9:   Solve for  $t$  such that  $(M - \lambda I_n)t = r$
  - 10:    $t := \Pi^{(j)} t$  ▷  $\Pi^{(j)}$  is a projector onto  $\text{range}(Q_j)^\perp$
  - 11:    $q_{j+1} := t / \|t\|_2$
-

## Generalized Davidson method, cont'd<sub>3</sub>

- For a **harmonic Ritz pair**  $(\lambda, y)$  with respect to a search space  $\text{range}(Q_k)$ , 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**  $j = 1, \dots, k$  **do**
- 4:    $w_j := (A - \sigma I_n) q_j$
- 5:    $G_1[1 : j, j] := W_j^H w_j$   $\triangleright G_1[j, 1 : j - 1] := G_1[1 : j - 1, j]^H$
- 6:    $G_2[1 : j, j] := Q_j^H w_j$ ,  $G_2 := [j, 1 : j - 1] := q_j^H W_{j-1}$
- 7:   Solve for eigenpair  $(\lambda, \hat{y})$  of  $G_2[1 : j, 1 : j]^{-H} G_1[1 : j, 1 : j]$  closest to 0
- 8:    $y := Q_j \hat{y}$ ,  $\delta_\rho := \hat{y}^H G_2 \hat{y}$ ,  $\rho := \sigma + \delta_\rho$ ,  $r := W_j \hat{y} - \delta_\rho y$
- 9:   Solve for  $t$  such that  $(M - \rho I_n)t = r$
- 10:    $t := \Pi^{(j)} t$ ,  $q_{j+1} := t / \|t\|_2$   $\triangleright \Pi^{(j)}$  is a projector onto  $\text{range}(Q_j)^\perp$

# 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  $(\alpha, e_1)$  is an **approximation** of the **largest eigenpair**  $(\theta, z)$  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  $\lambda_k$  is not a Rayleigh-Ritz value, it is nevertheless an approximation of the largest eigenvalue  $\theta$ .

► 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 (1996) 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

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

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

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

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

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

$$\begin{aligned} \text{is such that } (I_n - y_j y_j^H) (A - \theta I_n) \delta &= (I_n - y_j y_j^H) (-A y_j + \theta y_j) \\ &= - (I_n - y_j y_j^H) A y_j \\ &= - (A y_j - \vartheta_j y_j) =: -r_j. \end{aligned}$$

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  $\theta$ , which is **unknown**, is replaced by  $\vartheta_j$  to yield the **Jacobi-Davidson correction equation** given by:

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

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**.

# Exact solution of the Jacobi-Davidson correction equation

- The Jacobi-Davidson correction equation is such that

$$\begin{aligned}(I_n - y_j y_j^H)(A - \vartheta_j I_n)\delta &= -r_j, \quad \delta \perp y_j \\ (A - \vartheta_j I_n)\delta - y_j y_j^H(A - \vartheta_j I_n)\delta &= -r_j\end{aligned}$$

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  $\vartheta_j$  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  $\delta$  presented by Sleijpen and van der Vorst (1996), 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. Sauder (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. and van der Vorst, H. A. (1996). A Jacobi-Davidson iteration method for linear eigenvalue problems, SIAM J. Matrix Anal. Appl., 17 (1996), pp. 401-425.

# Jacobi-Davidson algorithm with Rayleigh-Ritz projections

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

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**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**  $j = 1, \dots, k$  **do**
  - 4:    $\tilde{t} := \Pi^{(j-1)} \tilde{t}$  ▷  $\Pi^{(j)}$  is a projector onto  $\text{range}(Q_j)^\perp$
  - 5:    $q_j := \tilde{t} / \|\tilde{t}\|_2$
  - 6:    $w_j := Aq_j$
  - 7:    $B_k[1 : j, j] := Q_j^H w_j, B_k[j, 1 : j - 1] := q_j^H W_{j-1}$
  - 8:   Solve for eigenpair  $(\lambda, \hat{y})$  of  $B_j$
  - 9:    $y := Q_j \hat{y}$
  - 10:    $r := W_j \hat{y}_j - \lambda y$
  - 11:   Solve for  $\tilde{t} \approx t$  such that  $(I_n - y_j y_j^H)(A - \lambda I_n)(I_n - y_j y_j^H) \tilde{t} = r$
-

# Jacobi-Davidson algorithm with harmonic Ritz projections

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

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**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**  $j = 1, \dots, k$  **do**
- 4:    $\tilde{t} := \Pi^{(j-1)} \tilde{t}$  ▷  $\Pi^{(j)}$  is a projector onto  $\text{range}(Q_j)^\perp$
- 5:    $q_j := \tilde{t} / \|\tilde{t}\|_2$
- 6:    $w_j := (A - \sigma I_n) q_j$
- 7:    $G_1[1 : j, j] := W_j^H w_j$  ▷  $G_1[j, 1 : j - 1] := G_1[1 : j - 1, j]^H$
- 8:    $G_2[1 : j, j] := Q_j^H w_j, G_2[j, 1 : j - 1] := q_j^H W_{j-1}$
- 9:   Solve for eigenpair  $(\lambda, \hat{y})$  of  $G_2[1:j, 1:j]^{-H} G_1[1:j, 1:j]$  closest to 0
- 10:    $y := Q_j \hat{y}$
- 11:    $\delta_\rho := \hat{y}^H G_2 \hat{y}, \rho := \sigma + \delta_\rho$
- 12:    $r := W_j \hat{y}_j - \delta_\rho y$
- 13:   Solve for  $\tilde{t} \approx t$  such that  $(I_n - y_j y_j^H)(A - \rho I_n)(I_n - y_j y_j^H) \tilde{t} = r$

# Homework problem



## Homework problem

Turn in **your own** solution to **Pb. 25**:

**Pb. 25** Show that if a matrix  $A \in \mathbb{F}^{n \times n}$  has constant diagonal components, i.e.,  $D_A \propto I_n$ , then, assuming exact arithmetic, the Davidson method is equivalent to applying a Rayleigh-Ritz projection to a Krylov subspace generated by a Arnoldi procedure with the same starting vector  $q$ .

# Practice session

## Practice session

- 1 Implement the MGS-based Davidson method with Rayleigh-Ritz projection to compute the most dominant eigenvalue of a matrix of your choice.
- 2 Implement the MGS-based generalized Davidson method with Rayleigh-Ritz projection to compute the most dominant eigenvalue of a matrix and the preconditioner of your choice.
- 3 Implement our basic MGS-based Davidson method with harmonic Ritz projection to compute an interior eigenpair of a matrix of your choice close to an arbitrary shift. What do you observe?
- 4 Implement the MGS-based generalized Davidson method with harmonic Ritz projection to compute an interior eigenpair of a matrix of your choice close to an arbitrary shift with a preconditioner of your choosing. What do you observe?
- 5 Implement an MGS-based Jacobi-Davidson method with Rayleigh-Ritz projection to compute a dominant eigenpair of a matrix of your choice using different numbers of solver iteration for the orthogonal correction equation.

## Practice session, cont'd

- 1 Implement an MGS-based Jacobi-Davidson method with harmonic Ritz projection to compute a dominant eigenpair of a matrix of your choice using different numbers of solver iteration for the orthogonal correction equation. What do you observe?