II.2 Quadratic eigenvalue problems

Basics

- The quadratic eigenvalue problem (QEP) is to find scalars λ and nonzero vectors x satisfying

$$Q(\lambda)x = 0, \tag{1}$$

  where

$$Q(\lambda) = \lambda^2 M + \lambda D + K,$$

  M, D and K are given $n \times n$ matrices.

- Sometimes, we are also interested in finding the left eigenvectors y:

$$y^H Q(\lambda) = 0.$$

- $Q(\lambda)$ has $2n$ eigenvalues λ. They are the roots of $\det[Q(\lambda)] = 0$.

Linearization

- A common way to solve the QEP is to first linearize it to a linear eigenvalue problem.
- For example, let

$$z = \begin{bmatrix} \lambda x \\ x \end{bmatrix},$$

Then the QEP (1) is equivalent to the generalized eigenvalue problem

$$L_c(\lambda) z = 0 \tag{2}$$

where

$$L_c(\lambda) = \lambda \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix} + \begin{bmatrix} D & K \\ -I & 0 \end{bmatrix} \equiv \lambda G + C.$$

$L_c(\lambda)$ is called a companion form or a linearization of $Q(\lambda)$.

- **Definition.** A matrix pencil $L(\lambda) = \lambda G + C$ is called a **linearization** of $Q(\lambda)$ if

$$E(\lambda)L(\lambda)F(\lambda) = \begin{bmatrix} Q(\lambda) & 0 \\ 0 & I \end{bmatrix} \qquad (3)$$

for some unimodular matrices $E(\lambda)$ and $F(\lambda)$.

- For the pencil $L_c(\lambda)$ in (2), the identity (3) holds with

$$E(\lambda) = \begin{bmatrix} I & \lambda M + D \\ 0 & -I \end{bmatrix}, \quad F(\lambda) = \begin{bmatrix} \lambda I & I \\ I & 0 \end{bmatrix}.$$

- There are various ways to linearize a QEP. Some are preferred than others. For example if M, D and K are symmetric and K is nonsingular, then we can preserve the symmetry property and use the following linearization:

$$L_c(\lambda) = \lambda \begin{bmatrix} M & 0 \\ 0 & K \end{bmatrix} + \begin{bmatrix} D & K \\ K & 0 \end{bmatrix}. \qquad (4)$$

- **Direct QEP method** (MATLAB's `polyeig(K,D,M)`).
  1. Linearize $Q(\lambda)$ into $L(\lambda) = \lambda G + C$.
  2. Solve the generalized eigenproblem $L(\lambda)z = 0$.
  3. Recover eigenvectors of Q from those of L.
- Additional issues on scaling and numerical sensitivity.

Arnoldi method

- Use the Arnoldi procedure to generate an orthonormal basis V_n of the Krylov subspace $\mathcal{K}_n(-G^{-1}C; -G^{-1}b)$, namely,

$$\begin{aligned} \text{span}\{V_n\} &= \mathcal{K}_n(-G^{-1}C; G^{-1}b) \\ &= \text{span}\{G^{-1}b, (-G^{-1}C)G^{-1}b, \ldots, (-G^{-1}C)^{n-1}G^{-1}b\} \end{aligned}$$

- The governing equation of the Arnoldi procedure is

$$(-G^{-1}C)\,V_n = V_{n+1}\widehat{H}_n, \tag{5}$$

where $\widehat{H}_n$ is an $(n+1) \times n$ upper Hessenberg matrix and V_{n+1} is a $2N \times (n+1)$ matrix with orthonormal columns.

- **Basic Arnoldi Method for Linearized QEP**
  1. Transform the QEP (1) to the equivalent generalized eigenvalue problem (2).
  2. Run the Arnoldi procedure with the matrix $H = -G^{-1}C$ and the vector $v = (\, u^T \; 0 \,)^T$ to generate an orthonormal basis $V_n = \{v_1, v_2, \ldots, v_n\}$ of $\mathcal{K}_n\,(H; v)$.
  3. Solve the reduced eigenvalue problem

     $$(V_n^T H V_n)t = \theta t,$$

     and obtain the Ritz pairs $(\theta, y = V_n t)$
  4. Extract the approximate eigenpairs $(\theta,\ z)$ of the QEP (1), and test their accuracy by the residual norms
- In practice, one may incorporate the implicit restarting scheme as we discussed for the standard Arnoldi procedure.

Q-Arnoldi method

- Note that
$$-G^{-1}C = \begin{bmatrix} -M^{-1}D & -M^{-1}K \\ I & 0 \end{bmatrix} = \begin{bmatrix} A & B \\ I & 0 \end{bmatrix}.$$
- Let us partition the jth Arnoldi vector v_j into
$$v_j = \begin{bmatrix} u_j \\ w_j \end{bmatrix}$$
where u_j and w_j are vectors of length n.
- From the second block row of the governing equation (5) of the Arnoldi procdure, we have
$$U_n = W_{n+1}\widehat{H}_n. \tag{6}$$

- Exploit this relation to avoid the storage of the U-vectors with a slight increase of computational cost, since all products with U_n are to be replaced by $W_{n+1}\widehat{H}_n$.
- Derive an Q-Arnoldi method with a simple replacement of the Arnoldi procedure by the Q-Arnoldi procedure at Step 2 of the Arnoldi algorithm.

Second-order Krylov subspace

- **Definition.** Let A and B be square matrices of order N, and $u \neq 0$ be an N-vector. Then the sequence

$$r_0, r_1, r_2, \ldots, r_{n-1}, \tag{7}$$

where

$$\begin{aligned} r_0 &= u, \\ r_1 &= Ar_0, \\ r_j &= Ar_{j-1} + Br_{j-2} \quad \text{for } j \geq 2, \end{aligned}$$

is called the **second-order Krylov sequence** of A, B on u. The space

$$\mathcal{G}_n(A, B; u) = \mathrm{span}\{r_0, r_1, r_2, \ldots, r_{n-1}\},$$

is called the n**th second-order Krylov subspace**.

- Motiviation
  - Recall that the QEP (1) $\Leftrightarrow$ generalized eigenvalue problem (2).
  - If one applies a Krylov subspace technique to (2), then an associated Krylov subspace would naturally be

$$\mathcal{K}_n(H; v) = \text{span}\left\{v, Hv, H^2v, \ldots, H^{n-1}v\right\}, \tag{8}$$

where v is a starting vector of length $2N$, and

$$H = -G^{-1}C = \begin{bmatrix} -M^{-1}D & -M^{-1}K \\ I & 0 \end{bmatrix} \equiv \begin{bmatrix} A & B \\ I & 0 \end{bmatrix} \tag{9}$$

then it immediately derives that the second-order Krylov vectors $\{r_j\}$ and the standard Krylov vectors $\{H^j v\}$ is related as the following form

$$\begin{bmatrix} r_j \\ r_{j-1} \end{bmatrix} = H^j v \quad \text{for } j \geq 1. \tag{10}$$

with $v = [u^{\mathrm{T}} \ \ 0]^{\mathrm{T}}$,

– In other words, the generalized Krylov sequence $\{r_j\}$ *defines* the entire standard Krylov sequence based on H and v.

Theorem. Let Q_n be an orthonormal basis of the second-order Krylov subspace $\mathcal{G}_n(A, B; u)$. Let $Q_{[n]}$ denote the following 2 by 2 block diagonal matrix

$$Q_{[n]} = \begin{pmatrix} Q_n & \\ & Q_n \end{pmatrix} \tag{11}$$

Then $H^\ell v \in \mathrm{span}\{Q_{[n]}\}$ for $\ell = 0, 1, 2, \ldots, n-1$. This means that

$$\mathcal{K}_n(H; v) \subseteq \mathrm{span}\{Q_{[n]}\}.$$

We call that the standard Krylov subspace $\mathcal{K}_n(H; \widehat{b}_0)$ is embedded into the second-order Krylov subspace $\mathcal{G}_n(A, B; r_0)$.

Second-Order ARnoldi (SOAR) procedure

- Construct an orthonormal basis $\{q_i\}$ of $\mathcal{G}_j(A, B; u)$:

$$\mathrm{span}\{q_1, q_2, \ldots, q_j\} = \mathcal{G}_j(A, B; u)$$

- **SOAR Procedure**

1. $q_1 = u/\|u\|_2$; $p_1 = 0$
2. **for** $j = 1, 2, \ldots, n$ **do**
3. $\quad r = Aq_j + Bp_j$; $s = q_j$
4. $\quad$ **for** $i = 1, 2, \ldots, j$ **do**
5. $\quad\quad t_{ij} = q_i^T r$
6. $\quad\quad r := r - q_i t_{ij}$; $s := s - p_i t_{ij}$
7. $\quad$ **end for**
8. $\quad t_{j+1\,j} = \|r\|_2$
9. $\quad$ **if** $t_{j+1\,j} = 0$, **stop**
10. $\quad q_{j+1} = r/t_{j+1\,j}$; $p_{j+1} = s/t_{j+1\,j}$
11. **end for**

Remark: The **for**-loop in Lines 4-7 is an orthogonalization procedure with respect to the $\{q_i\}$ vectors. The vector sequence $\{p_j\}$ is an auxiliary sequence.

- Let $Q_n = (q_1, q_2, \ldots, q_n),\ \ P_n = (p_1, p_2, \ldots, p_n),\ \ T_n = (t_{ij})_{n\times n}$. Note that T_n is upper Hessenberg. Then the following relations hold:

$$\begin{bmatrix} A & B \\ I & 0 \end{bmatrix} \begin{bmatrix} Q_n \\ P_n \end{bmatrix} = \begin{bmatrix} Q_{n+1} \\ P_{n+1} \end{bmatrix} \widehat{T}_n, \tag{12}$$

  where $Q_n^T Q_n = I_n$, and $\widehat{T}_n = \begin{bmatrix} T_n \\ e_n^T t_{n+1\,n} \end{bmatrix}$.

- This relation assembles the similarity between the SOAR procedure and the Arnoldi procedure.

  Theorem. If $t_{i+1,i} \neq 0$ for $i \leq j$, then the vector sequence $\{q_1, q_2, \ldots, q_j\}$ forms an orthonormal basis of the second-order Krylov subspace $\mathcal{G}_j\,(A, B; u)$:

$$\mathrm{span}\{Q_j\} = \mathcal{G}_j\,(A, B; u) \quad \text{for } j \geq 1. \tag{13}$$

- A variant of SOAR is to exploit the relations and reduce memory requirement and floating point operations by almost one half.

SOAR algorithm = RR + SOAR procedure

- Rayleigh-Ritz approximation procedure:

  seek an approximate eigenpair (θ, z), where $\theta \in \mathcal{C}$ and $z \in \mathcal{G}_n(A, B; u)$, by imposing the following Galerkin condition:

$$\left(\theta^2 M + \theta D + K\right) z \quad \perp \quad \mathcal{G}_n(A, B; u),$$

  or equivalently,

$$v^T \left(\theta^2 M + \theta D + K\right) z = 0 \quad \text{for all } v \in \mathcal{G}_n(A, B; u). \tag{14}$$

- Since $z \in \mathcal{G}_n(A, B; u)$, it can be written as $z = Q_m g$, where the $\mathrm{span} Q_m = \mathcal{G}_n(A, B; u)$

  By (14), it yields that θ and g must satisfy the reduced QEP:

$$\left(\theta^2 M_m + \theta D_m + K_m\right) g = 0 \tag{15}$$

  with $M_m = Q_m^T M Q_m$, $C_m = Q_m^T D Q_m$, $K_m = Q_m^T K Q_m$.

- The eigenpairs (θ, g) of (15) define the *Ritz pairs* $(\theta,\ z)$, approximate eigenpairs of the QEP (1).
- By explicitly formulating the matrices M_m, D_m and K_m, essential structures of M, D and K are preserved. As a result, essential spectral properties of the QEP will be preserved.

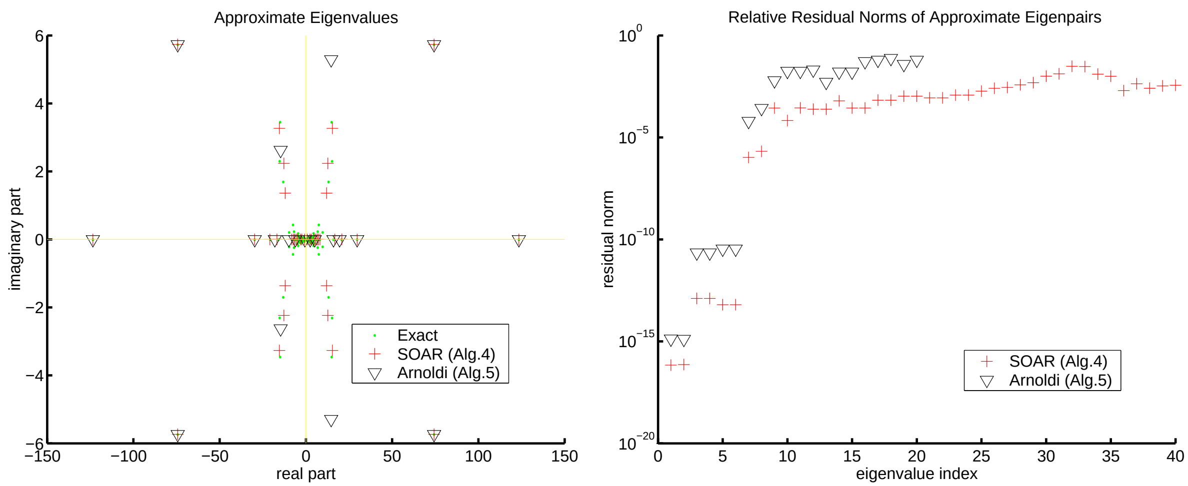
SOAR algorithm

1. Run SOAR procedure with $A = -M^{-1}D$ and $B = -M^{-1}K$ and a starting vector u to generate an $N \times m$ orthogonal matrix Q_m whose columns span an orthonormal basis of $\mathcal{G}_n(A, B; u)$.
2. Compute M_m, C_m and K_m
3. Solve the reduced QEP for (θ, g) and obtain the Ritz pairs (θ, z), where $z = Q_m g / \|Q_m g\|_2$.
4. Test the accuracy of Ritz pairs $(\theta,\ z)$ as approximate eigenvalues and eigenvectors of the QEP (1) by the relative norms of residual vectors:

$$\frac{\|(\theta^2 M + \theta D + K)z\|_2}{|\theta|^2\|M\|_1 + |\theta|\|C\|_1 + \|K\|_1} \tag{16}$$

An example to illusrate the benefits of structure-preservation

- An artifical gyroscopic dynamical system:
  $M^T = M > 0$, $C^T = -C$ and $K^T = K > 0$,
- The distribution of the eigenvalues of the system is symmetric with respect to both the real and imaginary axes.
- Eigenvalues and approximations relative residual norms.



- The SOAR method preserves the gyroscopic spectral property.