Polynomial Jacobi Davidson Method for Large/Sparse Eigenvalue Problems

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Outline

References

- SIAM J. Matrix Anal. Vol. 17, No. 2, PP. 401-425, 1996, Van der Vorst etc.
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Some basic theorems

Theorem 1

Let $\mathcal{X}$ be an eigenspace of A and let X be a basis for $\mathcal{X}$. Then there is a unique matrix L such that

$$AX = XL.$$

The matrix L is given by

$$L = X^I AX,$$

where X^I is a matrix satisfying $X^I X = I$.
If (λ, x) is an eigenpair of A with $x \in \mathcal{X}$, then $(\lambda, X^I x)$ is an eigenpair of L. Conversely, if (λ, u) is an eigenpair of L, then (λ, Xu) is an eigenpair of A.

Proof: Let

$$X = [x_1 \cdots x_k] \quad \text{and} \quad Y = AX = [y_1 \cdots y_k]\,.$$

Since $y_i \in \mathcal{X}$ and X is a basis for $\mathcal{X}$, there is a unique vector ℓ_i such that

$$y_i = X\ell_i.$$

If we set $L = [\ell_1 \cdots \ell_k]$, then $AX = XL$ and

$$L = X^I XL = X^I AX.$$

Now let (λ, x) be an eigenpair of A with $x \in \mathcal{X}$. Then there is a unique vector u such that $x = Xu$. However, $u = X^I x$. Hence

$$\lambda x = Ax = AXu = XLu \quad \Rightarrow \quad \lambda u = \lambda X^I x = Lu.$$

Conversely, if $Lu = \lambda u$, then

$$A(Xu) = (AX)u = (XL)u = X(Lu) = \lambda(Xu),$$

so that (λ, Xu) is an eigenpair of A.

Theorem 2 (Optimal residuals)

Let $[X \ X_\perp]$ *be unitary. Let*

$$R = AX - XL \quad \text{and} \quad S^H = X^H A - LX^H.$$

Then $\|R\|$ *and* $\|S\|$ *are minimized when*

$$L = X^H AX,$$

in which case

$$\begin{array}{ll} (a) & \|R\| = \|X_\perp^H AX\|, \\ (b) & \|S\| = \|X^H AX_\perp\|, \\ (c) & X^H R = 0. \end{array}$$

Proof: Set

$$\begin{bmatrix} X^H \\ X_\perp^H \end{bmatrix} A \begin{bmatrix} X & X_\perp \end{bmatrix} = \begin{bmatrix} \hat{L} & H \\ G & M \end{bmatrix}.$$

Then

$$\begin{bmatrix} X^H \\ X_\perp^H \end{bmatrix} R = \begin{bmatrix} \hat{L} & H \\ G & M \end{bmatrix} \begin{bmatrix} X^H \\ X_\perp^H \end{bmatrix} X - \begin{bmatrix} X^H \\ X_\perp^H \end{bmatrix} XL = \begin{bmatrix} \hat{L} - L \\ G \end{bmatrix}.$$

It implies that

$$\|R\| = \left\| \begin{bmatrix} X^H \\ X_\perp^H \end{bmatrix} R \right\| = \left\| \begin{bmatrix} \hat{L} - L \\ G \end{bmatrix} \right\|,$$

which is minimized when $L = \hat{L} = X^H AX$ and

$$\min \|R\| = \|G\| = \|X_\perp^H AX\|.$$

The proof for S is similar. If $L = X^H AX$, then

$$X^H R = X^H AX - X^H XL = X^H AX - L = 0.$$

Definition 3

Let X be of full column rank and let X^I be a left inverse of X. Then $X^I AX$ is a Rayleigh quotient of A.

Theorem 4

Let X be orthonormal, A be Hermitian and

$$R = AX - XL.$$

If $\ell_1, \ldots, \ell_k$ are the eigenvalues of L, then there are eigenvalues $\lambda_{j_1}, \ldots, \lambda_{j_k}$ of A such that

$$|\ell_i - \lambda_{j_i}| \leq \|R\|_2 \quad \textit{and} \quad \sqrt{\sum_{i=1}^{k} (\ell_i - \lambda_{j_i})^2} \leq \sqrt{2}\|R\|_F.$$

Jacobi's orthogonal component correction, 1846

Consider the eigenvalue problem

$$A \begin{bmatrix} 1 \\ z \end{bmatrix} \equiv \begin{bmatrix} \alpha & c^T \\ b & F \end{bmatrix} \begin{bmatrix} 1 \\ z \end{bmatrix} = \lambda \begin{bmatrix} 1 \\ z \end{bmatrix}, \qquad (1)$$

where A is diagonal dominant and α is the largest diagonal element. (1) is equivalent to

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

Jacobi iteration : (with $z_1 = 0$)

$$\begin{cases} \theta_k = \alpha + c^T z_k, \\ (D - \theta_k I) z_{k+1} = (D - F) z_k - b \end{cases} \qquad (2)$$

where $D = \text{diag}(F)$.

Davidson's method (1975)

Algorithm 1 (Davidson's method)

Given unit vector v, *set* $V = [v]$
Iterate until convergence
  Compute desired eigenpair (θ, s) *of* $V^T AV$.
  Compute $u = Vs$ *and* $r = Au - \theta u$.
  If $(\| r \|_2 < \varepsilon)$, *stop.*
  Solve $(D_A - \theta I)t = r$.
  Orthog. $t \perp V \rightarrow v, V = [V, v]$
end

Let $u_k = (1, z_k^T)^T$. Then

$$r_k = (A - \theta_k I)u_k = \begin{bmatrix} \alpha - \theta_k + c^T z_k \\ (F - \theta_k I)z_k + b \end{bmatrix}$$

Substituting the residual vector r_k into linear systems

$$(D_A - \theta_k I)t_k = -r_k, \quad \text{where} \quad D_A = \begin{bmatrix} \alpha & 0 \\ 0 & D \end{bmatrix},$$

we get

$$\begin{aligned} (D - \theta_k I)y_k &= -(F - \theta_k I)z_k - b \\ &= (D - F)z_k - (D - \theta_k I)z_k - b \end{aligned}$$

From (2) and above equality, we see that

$$(D - \theta_k I)(z_k + y_k) = (D - F)z_k - b = (D - \theta_k I)z_{k+1}.$$

This implies that $z_{k+1} = z_k + y_k$ as one step of JOCC starting with z_k.

Jacobi-Davidson method (1996)

(θ_k, u_k): approx. eigenpair of A, $\theta_k \approx \lambda$, with

$$u_k = V_k s_k,\ V_k^T A V_k s_k = \theta_k s_k \ \text{ and } \ \| s_k \|_2 = 1.$$

Definition 5

(θ_k, u_k) is called a Ritz pair of A. θ_k is called a Ritz value and u_k is a Ritz vector.

Jacobi-Davidson method (1996)

(θ_k, u_k): approx. eigenpair of A, $\theta_k \approx \lambda$, with

$$u_k = V_k s_k, \; V_k^T A V_k s_k = \theta_k s_k \text{ and } \| s_k \|_2 = 1.$$

Then

$$u_k^T r_k \equiv u_k^T (A - \theta_k I) u_k = s_k^T V_k^T A V_k s_k - \theta_k s_k^T V_k^T V_k s_k = 0 \;\Rightarrow\; r_k \perp u_k$$

Find the correction $t \perp u_k$ such that

$$A(u_k + t) = \lambda(u_k + t).$$

That is

$$(A - \lambda I)t = \lambda u_k - A u_k = -r_k + (\lambda - \theta_k) u_k.$$

Since $(I - u_k u_k^T) r_k = r_k$, we have

$$\left(I - u_k u_k^T\right)(A - \lambda I)t = -r_k.$$

Correction equation

$$(I - u_k u_k^T)(A - \theta_k I)\left(I - u_k u_k^T\right) t = -r_k \quad \text{and} \quad t \perp u_k,$$

Solving correction vector t

Correction equation:

$$\left(I - u_k u_k^T\right)(A - \theta_k I)(I - u_k u_k^T)t = -r_k, \quad t \perp u_k. \tag{3}$$

Scheme $\mathcal{S}_{OneLS}$:

- Use preconditioning iterative approximations, e.g., GMRES, to solve (3).
- Use a preconditioner

  $$\mathcal{M}_p \equiv \left(I - u_k u_k^T\right) \mathcal{M} \left(I - u_k u_k^T\right),$$

  where $\mathcal{M}$ is an approximation of $A - \theta_k I$.
- In each of the iterative steps, it needs to solve

  $$\mathcal{M}_p y = b, \quad y \perp u_k \tag{4}$$

  for a given b.

- Since $y \perp u_k$, Eq. (4) can be rewritten as

$$\left(I - u_k u_k^T\right) \mathcal{M} y = b \;\Rightarrow\; \mathcal{M} y = \left(u_k^T \mathcal{M} y\right) u_k + b \equiv \eta_k u_k + b.$$

Hence

$$y = \mathcal{M}^{-1} b + \eta_k \mathcal{M}^{-1} u_k,$$

where

$$\eta_k = -\frac{u_k^T \mathcal{M}^{-1} b}{u_k^T \mathcal{M}^{-1} u_k}.$$

- SSOR preconditioner: Let $A - \theta_k I = L + D + U$. Then

$$\mathcal{M} = (D + \omega L) D^{-1} (D + \omega U).$$

Scheme $\mathcal{S}_{TwoLS}$: Since $t \perp u_k$, Eq. (3) can be rewritten as

$$(A - \theta_k I)t = \left(u_k^T (A - \theta_k I)t\right) u_k - r_k \equiv \varepsilon u_k - r_k. \quad (5)$$

Let t_1 and t_2 be approximated solutions of the following linear systems:

$$(A - \theta_k I)t = -r_k \quad \text{and} \quad (A - \theta_k I)t = u_k,$$

respectively. Then the approximated solution $\tilde{t}$ for (5) is

$$\tilde{t} = t_1 + \varepsilon t_2 \quad \text{for} \quad \varepsilon = -\frac{u_k^T t_1}{u_k^T t_2}.$$

Scheme $\mathcal{S}_{OneStep}$: The approximated solution $\tilde{t}$ for (5) is

$$\tilde{t} = -\mathcal{M}^{-1} r_k + \varepsilon \mathcal{M}^{-1} u_k \quad \text{for} \quad \varepsilon = \frac{u_k^\top \mathcal{M}^{-1} r_k}{u_k^\top \mathcal{M}^{-1} u_k},$$

where $\mathcal{M}$ is an approximation of $A - \theta_k I$.

Algorithm 2 (Jacobi-Davidson Method)

Choose an n*-by-*m *orthonormal matrix* V_0

Do $k = 0, 1, 2, \cdots$

Compute all the eigenpairs of $V_k^T A V_k s = \lambda s$.

Select the desired (target) eigenpair (θ_k, s_k) *with* $\|s_k\|_2 = 1$.

Compute $u_k = V_k s_k$ *and* $r_k = (A - \theta_k I) u_k$.

If $(\|r_k\|_2 < \varepsilon)$, $\lambda = \theta_k$, $x = u_k$, *Stop*

Solve (approximately) a $t_k \perp u_k$ *from*

$$(I - u_k u_k^T)(A - \theta_k I)(I - u_k u_k^T)t = -r_k.$$

Orthogonalize $t_k \perp V_k \to v_{k+1}$, $V_{k+1} = [V_k, v_{k+1}]$

- Locking:
  V_k with $V_k^* V = I_k$ are convergent Schur vectors, i.e.,

$$AV_k = V_k T_k$$

  for some upper triangular T_k. Set $V = [V_k, V_q]$ with $V^* V = I_{k+q}$ in $k+1$-th iteration of Jacobi-Davidson Algorithm. Then

$$\begin{aligned} V^* AV &= \begin{bmatrix} V_k^* AV_k & V_k^* AV_q \\ V_q^* AV_k & V_q^* AV_q \end{bmatrix} = \begin{bmatrix} T_k & V_k^* AV_q \\ V_q^* V_k T_k & V_q^* AV_q \end{bmatrix} \\ &= \begin{bmatrix} T_k & V_k^* AV_q \\ 0 & V_q^* AV_q \end{bmatrix}. \end{aligned}$$

- Restarting:
  Keep the locked Schur vectors as well as the Schur vectors of interest in the subspace and throw away those we are not interested.

Remark 1

- *If $\varepsilon = 0$, we obtain Davidson method with*

$$t_1 = -(D_A - \theta_k I)^{-1} r.$$

($\tilde{t}$ is NOT orthogonal to u_k)

- *If the linear systems in (6) are exactly solved, then the vector t becomes*

$$t = \varepsilon (A - \theta_k I)^{-1} u_k - u_k. \tag{6}$$

Since t is made orthogonal to u_k, (6) is equivalent to

$$t = (A - \theta_k I)^{-1} u_k$$

which is equivalent to shift-invert power iteration. Hence it is quadratic convergence.

Consider $Ax = \lambda x$ and assume that λ is simple.

Lemma 6

Consider w with $w^T x \neq 0$. Then the map

$$F_p \equiv \left(I - \frac{xw^T}{w^T x} \right) (A - \lambda I) \left(I - \frac{xw^T}{w^T x} \right)$$

is a bijection from $w^\perp$ to $w^\perp$.

Proof: Suppose $y \perp w$ and $F_p y = 0$. That is

$$\left(I - \frac{xw^T}{w^T x} \right) (A - \lambda I) \left(I - \frac{xw^T}{w^T x} \right) y = 0.$$

Then it holds that

$$(A - \lambda I) y = \varepsilon x.$$

Therefore, both y and x belong to the kernel of $(A-\lambda I)^2$. The simplicity of λ implies that y is a scale multiple of x. The fact that $y \perp w$ and $x^T w \neq 0$ implies $y = 0$, which proves the injectivity of F_p. An obvious dimension argument implies bijectivity. $\square$

Extension

$$F_p t \equiv \left(I - \frac{uu^T}{u^T u}\right)(A-\theta I)\left(I - \frac{uu^T}{u^T u}\right) t = -r, \quad t \perp u, \; r \perp u.$$

Then

$$t \in u^\perp \underset{F_p}{\rightarrow} r \in u^\perp.$$

Theorem 7

Assume that the correction equation

$$\left(I - uu^T\right)(A - \theta I)\left(I - uu^T\right)t = -r, \quad t \perp u \tag{7}$$

is solved exactly in each step of Jacobi-Davidson Algorithm. Assume $u_k = u \to x$ and $u_k^T x$ has non-trivial limit. Then if u_k is sufficiently chosen to x, then $u_k \to x$ with locally quadratical convergence and

$$\theta_k = u_k^T A u_k \ \to\ \lambda.$$

Proof: Suppose $Ax = \lambda x$ with x such that $x = u + z$ for $z \perp u$. Then

$$(A - \theta I)\, z = -\,(A - \theta I)\, u + (\lambda - \theta)\, x = -r + (\lambda - \theta)\, x. \tag{8}$$

Consider the exact solution $z_1 \perp u$ of (7):

$$(I - P)\,(A - \theta I)\, z_1 = -\,(I - P)\, r, \tag{9}$$

where $P = uu^T$. Note that $(I - P)\, r = r$ since $u \perp r$. Since $x - (u + z_1) = z - z_1$ and $z = x - u$, for quadratic convergence, it suffices to show that

$$\|x - (u + z_1)\| = \|z - z_1\| = O\left(\|z\|^2\right). \tag{10}$$

Multiplying (8) by $(I - P)$ and subtracting the result from (9) yields

$$(I - P)\,(A - \theta I)\,(z - z_1) = (\lambda - \theta)\,(I - P)\, z + (\lambda - \theta)\,(I - P)\, u. \tag{11}$$

Multiplying (8) by u^T and using $r \perp u$ leads to

$$\lambda - \theta = \frac{u^T (A - \theta I) z}{u^T x}. \tag{12}$$

Since $u_k^T x$ has non-trivial limit, we obtain

$$\| (\lambda - \theta) (I - P) z \| = \left\| \frac{u^T (A - \theta I) z}{u^T x} (I - P) z \right\|. \tag{13}$$

From (11), Lemma 6 and $(I - P) u = 0$, we have

$$\begin{aligned} \| z - z_1 \| &= \left\| \left[(I - P) (A - \theta_k I) |_{u_k^\perp} \right]^{-1} (\lambda - \theta) (I - P) z \right\| \\ &= \left\| \left[(I - P) (A - \theta_k I) |_{u_k^\perp} \right]^{-1} \frac{u_k^T (A - \theta_k I) z}{u_k^T x} (I - P) z \right\| \\ &= O \left(\| z \|^2 \right). \end{aligned}$$

Jacobi Davidson method as on accelerated Newton Scheme

Consider $Ax = \lambda x$ and assume that λ is simple. Choose $w^T x = 1$.
Consider nonlinear equation

$$F(u) = Au - \theta(u)u = 0 \quad \text{with} \quad \theta(u) = \frac{w^T A u}{w^T u},$$

where $\|u\| = 1$ or $w^T u = 1$. Then $F : \{u | w^T u = 1\} \to w^\perp$. In particular, $r \equiv F(u) = Au - \theta(u)\, u \perp w$.
Suppose $u_k \approx x$ and the next Newton approximation u_{k+1}:

$$u_{k+1} = u_k - \left(\left. \frac{\partial F}{\partial u} \right|_{u=u_k} \right)^{-1} F(u_k)$$

is given by $u_{k+1} = u_k + t$, i.e., t satisfies that

$$\left(\left. \frac{\partial F}{\partial u} \right|_{u=u_k} \right) t = F(u_k) = -r.$$

Since $1 = u_{k+1}^T w = (u_k + t)^T w = 1 + t^T w$, it implies that $w^T t = 0$. By the definition of F, we have

$$\begin{aligned} \frac{\partial F}{\partial u} &= A - \theta(u) I - \frac{-\left(w^T A u\right) u w^T + \left(w^T u\right) u w^T A}{\left(w^T u\right)^2} \\ &= A - \theta I + \frac{w^T A u}{\left(w^T u\right)^2} u w^T - \frac{u w^T A}{w^T u} = \left(I - \frac{u_k w^T}{w^T u_k}\right)(A - \theta_k I). \end{aligned}$$

Consequently, the Jacobian of F acts on $w^{\perp}$ and is given by

$$\left(\left. \frac{\partial F}{\partial u} \right|_{u=u_k} \right) t = \left(I - \frac{u_k w^T}{w^T u_k}\right)(A - \theta_k I) t, \; t \perp w.$$

Hence the correction equation of Newton method read as

$$t \perp w, \quad \left(I - \frac{u_k w^T}{w^T u_k}\right)(A - \theta_k I) t = -r,$$

which is the correction equation of Jacobi-Davidson method in (7) with $w = u$.

Polynomial Jacobi-Davidson method

(θ_k, u_k): approx. eigenpair of $\mathbf{A}(\lambda) \equiv \sum_{k=0}^{\tau} \lambda^k A_k$, $\theta_k \approx \lambda$, with

$$u_k = V_k s_k, \; V_k^\top \mathbf{A}(\lambda) V_k s_k = 0 \;\text{ and }\; \| s_k \|_2 = 1.$$

Let

$$r_k = \mathbf{A}(\theta_k) u_k.$$

Then

$$u_k^\top r_k = u_k^\top \mathbf{A}(\theta_k) u_k = s_k^\top V_k^\top \mathbf{A}(\theta_k) V_k s_k = 0 \;\Rightarrow\; r_k \perp u_k$$

Find the correction t such that

$$\mathbf{A}(\lambda)(u_k + t) = 0.$$

That is

$$\mathbf{A}(\lambda) t = -\mathbf{A}(\lambda) u_k = -r_k + (\mathbf{A}(\theta_k) - \mathbf{A}(\lambda)) u_k.$$

Let

$$p_k = \mathbf{A}'(\theta_k)u_k \equiv \left(\sum_{i=1}^{\tau} i\theta_k^{i-1}A_i\right)u_k.$$

- $\mathbf{A}(\lambda) = A - \lambda I$:

$$\begin{aligned} p_k &= -u_k, \\ (\mathbf{A}(\theta_k) - \mathbf{A}(\lambda))u_k &= (\lambda - \theta_k)u_k = (\theta_k - \lambda_k)p_k \end{aligned}$$

- $\mathbf{A}(\lambda) = A - \lambda B$:

$$\begin{aligned} p_k &= -Bu_k, \\ (\mathbf{A}(\theta_k) - \mathbf{A}(\lambda))u_k &= (\lambda - \theta_k)Bu_k = (\theta_k - \lambda)p_k \end{aligned}$$

- $\mathbf{A}(\lambda) = \sum_{i=0}^{\tau} \lambda^i A_i$ with $\tau \geq 2$:

$$\begin{aligned} (\mathbf{A}(\theta_k) - \mathbf{A}(\lambda))u_k &= \left[(\theta_k - \lambda)\mathbf{A}'(\theta_k) - \frac{1}{2}(\theta_k - \lambda)^2\mathbf{A}''(\xi_k)\right]u_k \\ &= (\theta_k - \lambda)p_k - \frac{1}{2}(\theta_k - \lambda)^2\mathbf{A}''(\xi_k)u_k \end{aligned}$$

Hence

$$\mathbf{A}(\lambda)t = -r_k + (\theta_k - \lambda)p_k - \frac{1}{2}(\theta_k - \lambda)^2 \mathbf{A}''(\xi_k)u_k$$

Since $r_k \perp u_k$, we have

$$\left(I - \frac{p_k u_k^\top}{u_k^\top p_k}\right) \mathbf{A}(\lambda)t = -r_k - \frac{1}{2}(\theta_k - \lambda)^2 \left(I - \frac{p_k u_k^\top}{u_k^\top p_k}\right) \mathbf{A}''(\xi_k)u_k.$$

Correction equation:

$$\left(I - \frac{p_k u_k^\top}{u_k^\top p_k}\right) \mathbf{A}(\theta_k)(I - u_k u_k^\top)t = -r_k \text{ and } t \perp u_k,$$

or

$$\left(I - \frac{p_k u_k^\top}{u_k^\top p_k}\right) (A - \theta_k B) \left(I - \frac{u_k p_k^\top}{p_k^\top u_k}\right) t = -r_k \text{ and } t \perp_B u_k,$$

with symmetric positive definite matrix B.

Algorithm 3 (Jacobi-Davidson Algorithm for solving $\mathbf{A}(\lambda)x = 0$)

Choose an n*-by-*m *orthonormal matrix* V_0
Do $k = 0, 1, 2, \cdots$
  Compute all the eigenpairs of $V_k^\top \mathbf{A}(\lambda) V_k = 0$.
  Select the desired (target) eigenpair (θ_k, s_k) *with* $\|s_k\|_2 = 1$.
  Compute $u_k = V_k s_k$, $r_k = \mathbf{A}(\theta_k) u_k$ *and* $p_k = \mathbf{A}'(\theta_k) u_k$.
  If ($\|r_k\|_2 < \varepsilon$), $\lambda = \theta_k$, $x = u_k$, *Stop*
  Solve (approximately) a $t_k \perp u_k$ *from*

$$(I - \frac{p_k u_k^T}{u_k^T p_k}) \mathbf{A}(\theta_k)(I - u_k u_k^T) t = -r_k.$$

  Orthogonalize $t_k \perp V_k \to v_{k+1}$, $V_{k+1} = [V_k, v_{k+1}]$

$$p_k = \mathbf{A}'(\theta_k) u_k \equiv \left(\sum_{i=1}^{\tau} i \theta_k^{i-1} A_i \right) u_k.$$

Non-equivalence deflation of quadratic eigenproblems

Let λ_1 be a real eigenvalue of $\mathbf{Q}(\lambda) \equiv \lambda^2 M + \lambda C + K$ and x_1, z_1 be the associated right and left eigenvectors, respectively, with $z_1^T K x_1 = 1$. Let

$$\theta_1 = (z_1^T M x_1)^{-1}.$$

We introduce a deflated quadratic eigenproblem

$$\widetilde{\mathbf{Q}}(\lambda) x \equiv \left[\lambda^2 \widetilde{M} + \lambda \widetilde{C} + \widetilde{K}\right] x = 0,$$

where

$$\begin{aligned}
\widetilde{M} &= M - \theta_1 M x_1 z_1^T M, \\
\widetilde{C} &= C + \frac{\theta_1}{\lambda_1}(M x_1 z_1^T K + K x_1 z_1^T M), \\
\widetilde{K} &= K - \frac{\theta_1}{\lambda_1^2} K x_1 z_1^T K.
\end{aligned}$$

Complex deflation

Let $\lambda_1 = \alpha_1 + i\beta_1$ be a complex eigenvalue of $\mathbf{Q}(\lambda)$ and $x_1 = x_{1R} + ix_{1I}$, $z_1 = z_{1R} + iz_{1I}$ be the associated right and left eigenvectors, respectively, such that

$$Z_1^T K X_1 = I_2,$$

where $X_1 = [x_{1R}, x_{1I}]$ and $Z_1 = [z_{1R}, z_{1I}]$. Let

$$\Theta_1 = (Z_1^T M X_1)^{-1}.$$

Then we introduce a deflated quadratic eigenproblem with

$$\begin{aligned}
\widetilde{M} &= M - M X_1 \Theta_1 Z_1^T M, \\
\widetilde{C} &= C + M X_1 \Theta_1 \Lambda_1^{-T} Z_1^T K + K X_1 \Lambda_1^{-1} \Theta_1^T Z_1^T M, \\
\widetilde{K} &= K - K X_1 \Lambda_1^{-1} \Theta_1 \Lambda_1^{-T} Z_1^T K
\end{aligned}$$

in which $\Lambda_1 = \begin{bmatrix} \alpha_1 & \beta_1 \\ -\beta_1 & \alpha_1 \end{bmatrix}$.

Theorem 8

(i) *Let λ_1 be a simple real eigenvalue of $\mathbf{Q}(\lambda)$. Then the spectrum of $\widetilde{\mathbf{Q}}(\lambda)$ is given by*

$$(\sigma(\mathbf{Q}(\lambda))\diagdown\{\lambda_1\})\cup\{\infty\}$$

provided that $\lambda_1^2 \neq \theta_1$.

(ii) *Let λ_1 be a simple complex eigenvalue of $\mathbf{Q}(\lambda)$. Then the spectrum of $\widetilde{\mathbf{Q}}(\lambda)$ is given by*

$$\left(\sigma(\mathbf{Q}(\lambda))\diagdown\{\lambda_1,\bar{\lambda}_1\}\right)\cup\{\infty,\infty\}$$

provided that $\Lambda_1\Lambda_1^T \neq \Theta_1$.

Furthermore, in both cases (i) and (ii), if $\lambda_2 \neq \lambda_1$ and (λ_2, x_2) is an eigenpair of $\mathbf{Q}(\lambda)$ then the pair (λ_2, x_2) is also an eigenpair of $\widetilde{\mathbf{Q}}(\lambda)$.

Suppose that M, C, K are symmetric. Given an eigenmatrix pair $(\Lambda_1, X_1) \in \mathbb{R}^{r\times r} \times \mathbb{R}^{n\times r}$ of $Q(\lambda)$, where Λ_1 is nonsingular and X_1 satisfies

$$X_1^T K X_1 = I_r, \qquad \Theta_1 := (X_1^T M X_1)^{-1}.$$

We define $\tilde{Q}(\lambda) := \lambda^2 \tilde{M} + \lambda \tilde{C} + \tilde{K}$, where

$$\begin{aligned}
\tilde{M} &:= M - M X_1 \Theta_1 X_1^T M, \\
\tilde{C} &:= C + M X_1 \Theta_1 \Lambda_1^{-T} X_1^T K + K X_1 \Lambda_1^{-1} \Theta_1 X_1^T M, \\
\tilde{K} &:= K - K X_1 \Lambda_1^{-1} \Theta_1 \Lambda_1^{-T} X_1^T K.
\end{aligned}$$

Theorem 9

Suppose that $\Theta_1 - \Lambda_1 \Lambda_1^T$ is nonsingular. Then the eigenvalues of the real symmetric quadratic pencil $\tilde{Q}(\lambda)$ are the same as those of $Q(\lambda)$ except that the eigenvalues of Λ_1, which are closed under complex conjugation, are replaced by r infinities.

Proof: Since (Λ_1, X_1) is an eigenmatrix pair of $Q(\lambda)$, i.e.,

$$MX_1\Lambda_1^2 + CX_1\Lambda_1 + KX_1 = 0,$$

we have

$$\begin{aligned}\tilde{Q}(\lambda) &= Q(\lambda) + [MX_1(\lambda I_r + \Lambda_1) + CX_1]\,\Theta_1\Lambda_1^{-T}(X_1^TK - \lambda\Lambda_1^TX_1^TM) \\ &= Q(\lambda) + Q(\lambda)X_1(\lambda I_r - \Lambda_1)^{-1}\Theta_1\Lambda_1^{-T}(X_1^TK - \lambda\Lambda_1^TX_1^TM).\end{aligned}$$

By using the identity

$$\det(I_n + RS) = \det(I_m + SR),$$

where $R, S^T \in \mathbb{R}^{n\times m}$, we have

$$\begin{aligned}&\det[\tilde{Q}(\lambda)] \\ =\ &\det[Q(\lambda)]\det[I + X_1(\lambda I_r - \Lambda_1)^{-1}\Theta_1\Lambda_1^{-T}(X_1^TK - \lambda\Lambda_1^TX_1^TM)] \\ =\ &\det[Q(\lambda)]\det[I_r + (\lambda I_r - \Lambda_1)^{-1}\Theta_1\Lambda_1^{-T}(I_r - \lambda\Lambda_1^T\Theta_1^{-1})] \\ =\ &\frac{\det[Q(\lambda)]}{\det(\lambda I_r - \Lambda_1)}\det(\Theta_1\Lambda_1^{-T} - \Lambda_1).\end{aligned}$$

Since $(\Theta_1 - \Lambda_1 \Lambda_1^T) \in \mathbb{R}^{r \times r}$ is nonsingular, we have

$$\det(\Theta_1 \Lambda_1^{-T} - \Lambda_1) \neq 0.$$

Therefore, $\tilde{Q}(\lambda)$ has the same eigenvalues as $Q(\lambda)$ except that r eigenvalues of Λ_1 are replaced by r infinities. $\square$

Non-equiv. deflation for cubic poly. eigenproblems

Let $(\Lambda, V_u) \in \mathbb{R}^{r\times r} \times \mathbb{R}^{n\times r}$ be an eigenmatrix pair of

$$\mathbf{A}(\lambda) \equiv \lambda^3 A_3 + \lambda^2 A_2 + \lambda A_1 + A_0 \tag{14}$$

with $V_u^T V_u = I_r$ and $0 \notin \sigma(\Lambda)$, i.e.,

$$A_3 V_u \Lambda^3 + A_2 V_u \Lambda^2 + A_1 V_u \Lambda + A_0 V_u = 0. \tag{15}$$

Define a new deflated cubic eigenvalue problem by

$$\widetilde{\mathbf{A}}(\lambda) u = (\lambda^3 \tilde{A}_3 + \lambda^2 \tilde{A}_2 + \lambda \tilde{A}_1 + \tilde{A}_0) u = 0, \tag{16}$$

where

$$\begin{cases} \tilde{A}_0 = A_0, \\ \tilde{A}_1 = A_1 - (A_1 V_u V_u^T + A_2 V_u \Lambda V_u^T + A_3 V_u \Lambda^2 V_u^T), \\ \tilde{A}_2 = A_2 - (A_2 V_u V_u^T + A_3 V_u \Lambda V_u^T), \\ \tilde{A}_3 = A_3 - A_3 V_u V_u^T. \end{cases} \tag{17}$$

Lemma 10

Let $\mathbf{A}(\lambda)$ *and* $\widetilde{\mathbf{A}}(\lambda)$ *be cubic pencils given by (14) and (16), respectively. Then it holds*

$$\widetilde{\mathbf{A}}(\lambda) = \mathbf{A}(\lambda)\left(I_n - \lambda V_u(\lambda I_r - \Lambda)^{-1}V_u^T\right). \tag{18}$$

Theorem 11

Let (Λ, V_u) *be an eigenmatrix pair of* $\mathbf{A}(\lambda)$ *with* $V_u^T V_u = I_r$. *Then*

(i) $(\sigma(\mathbf{A}(\lambda)) \setminus \sigma(\Lambda)) \cup \{\infty\} = \sigma(\widetilde{\mathbf{A}}(\lambda))$.

(ii) *Let* (μ, z) *be an eigenpair of* $\mathbf{A}(\lambda)$ *with* $\| z \|_2 = 1$ *and* $\mu \notin \sigma(\Lambda)$. *Define*

$$\tilde{z} = (I_n - \mu V_u \Lambda^{-1} V_u^T)z \equiv T(\mu)z. \tag{19}$$

Then $(\mu, \tilde{z})$ *is an eigenpair of* $\widetilde{\mathbf{A}}(\lambda)$.

Proof of Lemma: Using (17) and (15), and the fundamental matrix calculation, we have

$$
\begin{aligned}
\widetilde{\mathbf{A}}(\lambda) &= \mathbf{A}(\lambda) - \lambda\left(\lambda^2 A_3 V_F V_F^T + \lambda A_2 V_F V_F^T + \lambda A_3 V_F \Lambda V_F^T\right. \\
&\quad \left. + A_1 V_F V_F^T + A_2 V_F \Lambda V_F^T + A_3 V_F \Lambda^2 V_F^T\right) \\
&= \mathbf{A}(\lambda) - \lambda\left(A_3 V_F (\lambda I_r - \Lambda)^3 (\lambda I_r - \Lambda)^{-1} V_F^T\right. \\
&\quad + 3A_3 V_F \Lambda (\lambda I_r - \Lambda)^2 (\lambda I_r - \Lambda)^{-1} V_F^T \\
&\quad + 3A_3 V_F \Lambda^2 (\lambda I_r - \Lambda)(\lambda I_r - \Lambda)^{-1} V_F^T \\
&\quad + A_2 V_F (\lambda I_r - \Lambda)^2 (\lambda I_r - \Lambda)^{-1} V_F^T \\
&\quad + 2A_2 V_F \Lambda (\lambda I_r - \Lambda)(\lambda I_r - \Lambda)^{-1} V_F^T \\
&\quad \left. + A_1 V_F (\lambda I_r - \Lambda)(\lambda I_r - \Lambda)^{-1} V_F^T\right)
\end{aligned}
$$

$$
\begin{aligned}
\widetilde{\mathbf{A}}(\lambda) &= \mathbf{A}(\lambda) - \lambda \left\{ \left[A_3 V_F(\lambda^3 I_r - \Lambda^3) + A_2 V_F(\lambda^2 I_r - \Lambda^2) \right.\right. \\
&\quad \left.\left. + A_1 V_F(\lambda I_r - \Lambda) + A_0 V_F - A_0 V_F \right] (\lambda I_r - \Lambda)^{-1} V_F^T \right\} \\
&= \mathbf{A}(\lambda) - \lambda \left[\mathbf{A}(\lambda) V_F (\lambda I_r - \Lambda)^{-1} V_F^T \right] \\
&= \mathbf{A}(\lambda) \left[I_n - \lambda V_F (\lambda I_r - \Lambda)^{-1} V_F^T \right].
\end{aligned}
$$

$\square$

Proof of Theorem: (i) Using the identity

$$\det(I_n + RS) = \det(I_m + SR)$$

and Lemma 10, we have

$$\begin{aligned}
\det(\widetilde{\mathbf{A}}(\lambda)) &= \det(\mathbf{A}(\lambda)) \det\left(I_n - \lambda V_F(\lambda I_r - \Lambda)^{-1} V_F^T\right) \\
&= \det(\mathbf{A}(\lambda)) \det\left(I_n - \lambda(\lambda I_r - \Lambda)^{-1}\right) \\
&= \det(\mathbf{A}(\lambda)) \det(\lambda I_r - \Lambda)^{-1} \det(-\Lambda).
\end{aligned}$$

Since $0 \notin \sigma(\Lambda)$, $\det(-\Lambda) \neq 0$. Thus, $\widetilde{\mathbf{A}}(\lambda)$ and $\mathbf{A}(\lambda)$ have the same finite spectrum except the eigenvalues in $\sigma(\Lambda)$. Furthermore, dividing Eq. (16) by λ^3 and using the fact that

$$\widetilde{\mathbf{A}}_3 V_F = (A_3 - A_3 V_F V_F^T) V_F = 0,$$

we see that $(\text{diag}_r\{\infty, \cdots, \infty\}, V_F)$ is an eigenmatrix pair of $\widetilde{\mathbf{A}}(\lambda)$ corresponding to infinite eigenvalues.

(ii) Since $\mu \notin \sigma(\Lambda)$, the matrix $T(\mu) = (I - \mu V_F \Lambda^{-1} V_F^T)$ in (19) is invertible with the inverse

$$T(\mu)^{-1} = I_n - \mu V_F (\mu I_r - \Lambda)^{-1} V_F^T. \tag{20}$$

From Lemma 10, we have

$$\widetilde{\mathbf{A}}(\mu)\tilde{z} = \mathbf{A}(\mu)\left[I_n - \mu V_F(\mu I_r - \Lambda)^{-1} V_F^T\right]\left[I_n - \mu V_F \Lambda^{-1} V_F^T\right] z = 0.$$

This completes the proof. $\square$