Palindromic cyclic reduction and matrix functions

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Advanced Workshop on Matrix Geometries and Applications
ICTP, Trieste, July 9–12, 2013

Quadratic palindromic matrix polynomials

In the recent literature there are several definitions of palindromic matrix polynomials ($*$-palindromic, T-palindromic,...).

In our setting a quadratic palindromic matrix polynomial is

$$\varphi(z) = Pz^2 + Qz + P$$

where P and Q are $n \times n$ matrices.

Throughout we assume that Q is nonsingular.

Spectral properties

Observe that $\varphi(z^{-1}) = Pz^{-2} + Qz^{-1} + P = z^{-2}\varphi(z)$.

Therefore, if $\lambda \in \mathbb{C}$, $\lambda \neq 0$ and $x \in \mathbb{C}^n$, $x \neq 0$, are such that $\varphi(\lambda)x = 0$, then $\varphi(\lambda^{-1})x = 0$.

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Hence, with the convention that $1/0 = \infty$ and $1/\infty = 0$:

- the roots of $\varphi(z)$ come to pairs $(\lambda, 1/\lambda)$;
- if $\det(\varphi(z)) \neq 0$ for $|z| = 1$, then $\varphi(z)$ has exactly n roots in the open unit disk, and n roots outside the closed unit disk, i.e., the roots of $\varphi(z)$ have a splitting with respect to the unit circle.

Under which conditions do the roots of $\varphi(z)$ have a splitting with respect to the unit circle?

Spectral properties – cont.

- The roots of $\varphi(z)$ have a splitting with respect to the unit circle if and only if the real eigenvalues of $M = Q^{-1}P$ belong to $(-1/2, 1/2)$.

Spectral properties – cont.

- The roots of $\varphi(z)$ have a splitting with respect to the unit circle if and only if the real eigenvalues of $M = Q^{-1}P$ belong to $(-1/2, 1/2)$.
- To each real eigenvalue of M of modulus $1/2$, there corresponds a root of multiplicity 2 of $\varphi(z)$, equal to ± 1.
- To each real eigenvalue of M, lying outside the interval to $[-1/2, 1/2]$, there correspond two distinct roots on the unit circle of $\varphi(z)$.

Laurent matrix polynomials

Let $\mathcal{L}(z) = Pz^{-1} + Q + Pz$ and assume that the real eigenvalues of M belong to the interval $(-1/2, 1/2)$.
Then:

- $\mathcal{L}(z)$ is invertible in the annulus $\mathcal{A}_R = \{z \in \mathbb{C} : \; R < |z| < 1/R\}$, where $R = \rho(X_*) < 1$, and $X_* = -2M(I + (I - 4M^2)^{1/2})^{-1}$ solves $P + QX + PX^2 = 0$
- $\mathcal{L}(z)$ can be factorized as

$$\mathcal{L}(z) = (I - QX_* Q^{-1} z)(Q + PX_*)(I - X_* z^{-1}), \quad z \in \mathcal{A}_R$$

- if $\mathcal{H}(z) = \mathcal{L}(z)^{-1} = H_0 + \sum_{i=1}^{+\infty} H_i(z^i + z^{-i})$, we have

$$H_0 = (I - 4M^2)^{-1/2} Q^{-1}$$

Matrix square root

Let A be a square matrix without real nonpositive eigenvalues. The principal matrix square root $A^{1/2}$ is the unique solution of

$$X^2 - A = 0$$

having eigenvalues with positive real part.

The definition is extended to the case where A does not have negative real eigenvalues and the null eigenvalue is semisimple.

Matrix sign

Let A be a square matrix without pure imaginary eigenvalues, and let

$$J = V^{-1}AV = \begin{bmatrix} J_- & 0 \\ 0 & J_+ \end{bmatrix}$$

its Jordan normal form, where $\sigma(J_-) \in \mathbb{C}_-$, $\sigma(J_+) \in \mathbb{C}_+$.
The matrix sign of A is defined as

$$\mathrm{sign}(A) = V \begin{bmatrix} -I_p & 0 \\ 0 & I_q \end{bmatrix} V^{-1}$$

where $p = \mathrm{size} J_-$ and $q = \mathrm{size} J_+$.

Matrix polar factor

Let A be a square nonsingular matrix.
The unitary polar factor, denoted by $\mathrm{polar}(A)$, is the unique matrix U such that

$$A = UH, \quad U^*U = I,$$

where H is Hermitian positive definite.

Geometric matrix mean

Let A and B be hermitian positive definite.
The matrix geometric mean between A and B is

$$A\#B = A^{1/2}(A^{-1/2}BA^{-1/2})^{1/2}A^{1/2}$$

Matrix functions and palindromic Laurent polynomials

Assume that

$$\mathcal{L}(z) = \frac{1}{4}(S - T)z^{-1} + \frac{1}{2}(S + T) + \frac{1}{4}(S - T)z$$

Matrix functions and palindromic Laurent polynomials

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The following properties hold:

1. If A does not have nonpositive real eigenvalues, $S = I$, $T = A^{-1}$, then $H_0 = A^{1/2}$.

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2. If A does not have imaginary eigenvalues, $S = A^{-1}$, $T = A$, then $H_0 = \mathrm{sign}(A)$.
3. If $\det A \neq 0$, $S = A^{-1}$, $T = A^*$, then $H_0 = \mathrm{polar}(A)$.

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3. If $\det A \neq 0$, $S = A^{-1}$, $T = A^*$, then $H_0 = \mathrm{polar}(A)$.
4. If $A > 0$, $B > 0$, $S = A^{-1}$ and $T = B^{-1}$, then $H_0 = A \# B$.

Cyclic reduction (CR)

CR is a versatile algorithm invented by G. Golub [Buzbee, Golub, Nielson 1970] for the f.d. Poisson equation.
Given $A_0, A_1, A_2 \in \mathbb{R}^{N\times N}$ such that the roots of $\varphi(z) = \det(A_0 + A_1 z + A_2 z^2)$ are

$$|\xi_1| \le \cdots \le |\xi_N| < 1 < |\xi_{N+1}| \le \cdots \le |\xi_{2N}|,$$

including zeros at ∞ if $\deg\varphi(\lambda) < 2N$, CR generates the matrix sequences

$$\begin{aligned} A_0^{(k+1)} &= -A_0^{(k)} S^{(k)} A_0^{(k)}, \quad S^{(k)} = (A_1^{(k)})^{-1} \\ A_2^{(k+1)} &= -A_2^{(k)} S^{(k)} A_2^{(k)}, \\ A_1^{(k+1)} &= A_1^{(k)} - A_0^{(k)} S^{(k)} A_2^{(k)} - A_2^{(k)} S^{(k)} A_0^{(k)}, \quad k \ge 0 \end{aligned}$$

starting from $A_i^{(0)} = A_i$, $i = 1, 2, 3$.

Functional formulation of CR

Let

$$\varphi_k(z) = A_0^{(k)} + A_1^{(k)} z + A_2^{(k)} z^2,$$

$$\psi_k(z) = z\varphi_k(z)^{-1}, \quad k = 0, 1, \ldots$$

Then, for any $k \geq 0$,

$$\varphi_{k+1}(z^2) = \varphi_k(z) \left(A_1^{(k)}\right)^{-1} \varphi_k(-z) \;\; \text{(Graeffe iteration)}$$

$$\psi_{k+1}(z^2) = \tfrac{1}{2}(\psi_k(z) + \psi_k(-z))$$

Properties of CR

Applicability: under mild conditions the matrices $A_1^{(k)}$ are invertible

Convergence property: the convergence is quadratic, more specifically:

$$||A_1^{(k)} - A_1^*|| = O(|\xi_N/\xi_{N+1}|^{2^k}),$$

$$||A_0^{(k)}|| = O(|\xi_N|^{2^k}), \quad ||A_2^{(k)}|| = O(|1/\xi_{N+1}|^{2^k})$$

Critical case: Under mild conditions, if $|\xi_N| = |\xi_{N+1}| = 1$ convergence turns to linear with rate $1/2$.

Convergence properties

If $|\xi_N| < 1 < |\xi_{N+1}|$ then:

- $\psi(z) = A_0 z^{-1} + A_1 + A_2 z$ is invertible in an annulus containing the unit circle and, setting $H(z) = \psi(z)^{-1} = \sum_{i=-\infty}^{+\infty} H_i z^i$, we have

$$\lim_k A_1^{(k)} = H_0^{-1}$$

- if the matrix equation $A_0 + A_1 X + A_2 X^2 = 0$ has a solution G with $\rho(G) < 1$, the sequence

$$\widehat{A}^{(k+1)} = \widehat{A}^{(k)} - A_0^{(k)} S^{(k)} A_2^{(k)}, \quad k \geq 0,$$

with $\widehat{A}^{(0)} = A_1$ is such that

$$\lim_k (-\widehat{A}^{(k)})^{-1} A_0 = G$$

Palindromic cyclic reduction (PCR)

Cyclic reduction applied to $\varphi(z) = Pz^2 + Qz + P$ generates the sequences

$$\begin{cases} P_0 = P, \quad Q_0 = Q, \\ P_{k+1} = -P_k Q_k^{-1} P_k, \\ Q_{k+1} = Q_k - 2P_k Q_k^{-1} P_k, \qquad k = 0, 1, 2, \ldots \end{cases}$$

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By setting $X_k = Q_k$ and $H_k = 2P_{k+1}$, PCR can be rewritten as

$$\begin{cases} X_0 = Q, \quad H_0 = -2PQ^{-1}P \\ X_{k+1} = X_k + H_k, \\ H_{k+1} = -\frac{1}{2}(H_k X_{k+1}^{-1} H_k), \qquad k = 0, 1, 2, \ldots. \end{cases} \tag{1}$$

Remark: The recursive expression for X_k looks like Newton's method, where H_k is the Newton increment.

Newton's method

If A admits the principal square root, Newton's method applied to compute $A^{1/2}$ is:

$$Y_{k+1} = \frac{1}{2}(Y_k + AY_k^{-1}), \quad k = 0, 1, \ldots, \quad Y_0 = I$$

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Connection with PCR: Set $M = Q^{-1}P$ and $A = I - 4M^2$.
Then

$$X_k = QY_k, \quad H_k = Q(Y_{k+1} - Y_k), \quad k = 0, 1, \ldots.$$

Therefore, up to the multiplication by Q, PCR and Newton's method generate the same matrix sequence

A three-term recurrence

Recurrences (1) can be expressed in terms of the matrices X_k, $k \geq 0$, only. Indeed, we find that

$$X_{k+1} = X_k + H_k = X_k - \frac{1}{2} H_{k-1} X_k^{-1} H_{k-1}$$

$$= X_k - \frac{1}{2}(X_k - X_{k-1}) X_k^{-1} (X_k - X_{k-1}) = \frac{1}{2}(X_k + 2X_{k-1} - X_{k-1} X_k^{-1} X_{k-1}).$$

The resulting iteration is the three-term recurrence

$$X_{k+1} = \frac{1}{2}(X_k + 2X_{k-1} - X_{k-1} X_k^{-1} X_{k-1}), \quad k = 1, 2, \ldots,$$

with $X_0 = Q$, $X_1 = Q - 2PQ^{-1}P$.

A formulation with commuting matrices

By setting $Y_k = X_{k-1}X_k^{-1}$, we find that

$$Y_{k+1} = \frac{1}{2}\left(I + 2Y_k^{-1} - (Y_k^{-1})^2\right), \quad k = 0, 1, 2, \ldots,$$

starting with $Y_0 = I - 2(PQ^{-1})^2$.
If we introduce also the matrix sequence

$$Z_{k+1} = Y_k Z_k, \quad k = 0, 1, 2, \ldots,$$

with $Z_0 = Q$, we find that $Z_k = X_k$ for any $k \geq 0$.

Therefore the sequences $\{Y_k\}_k$ and $\{Z_k\}_k$ represent another formulation of PCR.

The matrices Y_k, $k \geq 0$, commute each other and, in the case of convergence of PCR, converge to the identity matrix.

PCR and Gauss-Chebyshev quadrature

From the Cauchy integral formula one has

$$H_0 = \frac{1}{\pi}\int_{-1}^{1} \frac{(Q+2Pt)^{-1}}{\sqrt{1-t^2}}dt.$$

The Gauss-Chebyshev quadrature with k nodes is

$$C_k = \frac{1}{k}\sum_{j=0}^{k-1}\left(Q + 2P\cos\frac{(2j+1)\pi}{2k}\right)^{-1}.$$

and

$$C_{2^k} = Q_k^{-1}.$$

The k-th step of PCR is equivalent to G-C quadrature with 2^k knots

Trapezoidal rule

A change of variable leads to

$$H_0 = \frac{1}{\pi}\int_0^\pi (Q + 2P\cos\theta)^{-1}\, d\theta.$$

The trapezoidal rule with $k+1$ knots yields

$$T_k = \frac{1}{k}\left[\frac{(Q+2P)^{-1}}{2} + \sum_{j=1}^{k-1}\left(Q + 2P\cos\frac{\pi j}{k}\right)^{-1} + \frac{(Q-2P)^{-1}}{2}\right]$$

PCR and averaging technique

One has

$$T_{2^{k+1}} = \frac{1}{2}(T_{2^k} + C_{2^k}), \quad C_{2^{k+1}} = 2(C_{2^k}^{-1} + T_{2^k}^{-1})^{-1}$$

therefore the resulting iteration is

$$\begin{cases} A_1 = \frac{1}{2}\left((Q+2P)^{-1} + (Q-2P)^{-1}\right), \quad B_1 = Q^{-1}, \\ A_{k+1} = \frac{1}{2}(A_k + B_k), \\ B_{k+1} = 2A_k(A_k + B_k)^{-1}B_k, \quad k = 1, 2, \ldots, \end{cases}$$

where $B_k = Q_k^{-1}$ and $\lim_k A_k = \lim_k B_k = \lim_k Q_k^{-1} = H_0$.

Scaling technique

$$\begin{cases} X_0 = Q, \quad H_0 = -2PQ^{-1}P, \\ \gamma_k = \left| \dfrac{\det(X_k)^2}{\det(I - 4M^2)\det(Q)^2} \right|^{-1/(2n)}, \\ \widehat{X}_k = \gamma_k X_k, \qquad \widehat{H}_k = \gamma_k^{-1}(H_k + X_k/2) - \gamma_k X_k/2, \\ X_{k+1} = \widehat{X}_k + \widehat{H}_k, \qquad H_{k+1} = -\dfrac{1}{2}(\widehat{H}_k X_{k+1}^{-1} \widehat{H}_k), \qquad k = 0, 1, 2, \ldots. \end{cases}$$

The parameter γ_k is obtained at no additional cost during the inversion of X_k.

In certain cases the convergence is dramatically accelerated

PCR: convergence properties

The following properties hold:

1. PCR is well defined and convergent if and only if the real eigenvalues of M belong to the interval $[-1/2, 1/2]$, and the real eigenvalues of modulus $1/2$ (if any) are semisimple.

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   $P_k \to 0, \quad Q_k \to Q(1 - 4M^2)^{1/2} = H_0^{-1}$

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1. PCR is well defined and convergent if and only if the real eigenvalues of M belong to the interval $[-1/2, 1/2]$, and the real eigenvalues of modulus $1/2$ (if any) are semisimple.
2. If PCR is convergent then
   $P_k \to 0, \quad Q_k \to Q(1 - 4M^2)^{1/2} = H_0^{-1}$
3. The convergence is:
   - quadratic if the real eigenvalues of M belong to the interval $(-1/2, 1/2)$;
   - linear if M has at least one semisimple eigenvalue equal to $\pm 1/2$.

PCR and $A^{1/2}$, $\mathrm{sign}(A)$, $\mathrm{polar}(A)$, $A\#B$

Let $P = \frac{1}{4}(B - A)$ and $Q = \frac{1}{2}(B + A)$. Then, given the matrices A and B, chosen according to the table below, the sequence Q_k converges to the corresponding matrix function.

A	B	$\lim_k Q_k$
$\sigma(A) \cap \mathbb{R}_- = \emptyset$	I	$A^{1/2}$
$\sigma(A) \cap \mathbb{C}_0 = \emptyset$	A^{-1}	$\mathrm{sign}(A)$
$\det(A) \neq 0$	A^{-*}	$\mathrm{polar}(A)$
$A > 0$	$B > 0$	$A\#B$

Numerical experiments

Set $P = \frac{1}{4}(B_\epsilon - A_\epsilon)$, $Q = \frac{1}{2}(A_\epsilon + B_\epsilon)$, where A_ϵ, B_ϵ are $n \times n$ symmetric positive definite, depending on $0 < \epsilon < \frac{1}{2}$, such that $M = Q^{-1}P$ has eigenvalues

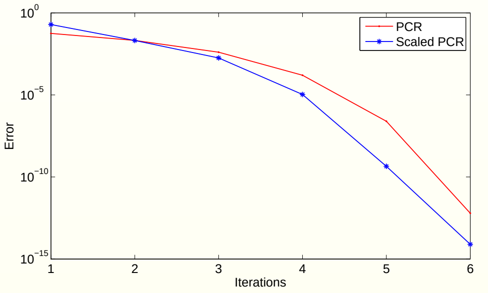
$$\frac{1}{2} - \epsilon, \frac{1}{3}, \ldots, \frac{1}{n+1}$$

Under these assumptions

$$\lim_k Q_k = A_\epsilon \# B_\epsilon$$

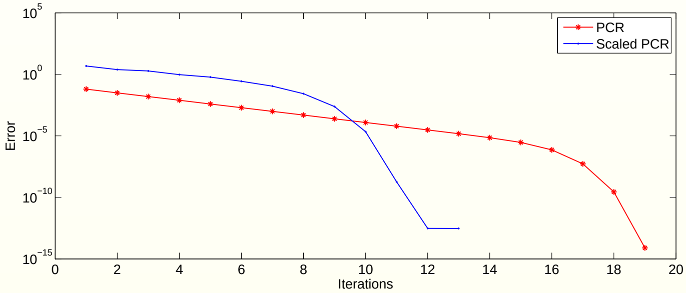
$n = 10$, $\epsilon =$ 1.e-5

	Absolute err.	Relative err.
PCR	2.0e-14	5.4e-15
Commuting mat.	2.3e-14	6.2e-15
3-term iter	9.6e-13	1.7e-14
Scaled PCR	1.7e-14	3.0e-15



$n = 10$, $\epsilon =$1.e-10

	Absolute err.	Relative err.
PCR	6.4e-12	1.7e-12
Commuting mat.	8.3e-12	2.2e-12
3-term iter	8.1e-10	1.9e-10
Scaled PCR	4.1e-12	7.3e-13



Open issues

- We have related palindromic quadratic matrix polynomials with $A^{1/2}$, $\mathrm{sign}(A)$, $\mathrm{polar}(A)$, $A\#B$. Are there any other matrix functions related to these polynomials?
- Can the theory developed for palindromic CR be extended to general CR? In particular, necessary and sufficient conditions for convergence, scaling technique, can be given for general CR?