A Padé family of iterations for $sign(A)$ and $sect_p(A)$ and related problems

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- **Laszkiewicz, Ziętak,** A Padé family of iterations for the matrix sector function and the matrix pth root,
  Numer. Lin. Alg. Appl. (2009).
- **Gomilko, Greco, Ziętak,** A Padé family of iterations for the matrix sign function and related problems,
  Numer. Lin. Alg. Appl. (2011).
- **Gomilko, Karp, Lin, Ziętak,** Regions of convergence of a Padé family of iterations for the matrix sector function,
  J. Comput. Appl. Math. (2012).

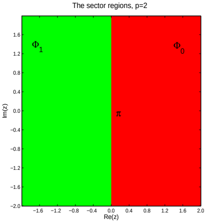
Outline

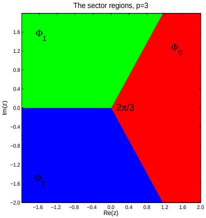
1. Sign and sector functions
2. Padé iterations
3. Structure-preserving matrix iterations
4. Convergence
5. Padé approximants
6. Open problems
7. References

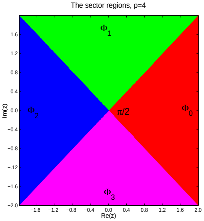
Sector regions - p integer

$$\Phi_k = \left\{ z \in \mathbb{C} : \frac{2k\pi}{p} - \frac{\pi}{p} < \arg(z) < \frac{2k\pi}{p} + \frac{\pi}{p} \right\}$$

$k = 0, \ldots, p-1$







Scalar p-sector function

$\mathrm{sect}_p(z)$ is the nearest *pth* root of unity to z

$$\mathrm{sect}_p(z) = \frac{z}{\sqrt[p]{z^p}}$$

$\mathrm{sect}_p(z)$ lies in the sector Φ_k in which z is

$p = 2 \quad$ sign function

Matrix sector function
Shieh, Tsay, Wang (1984)

$$\mathrm{sect}_p A = A \left(\sqrt[p]{A^p} \right)^{-1}$$

Matrix sign function
Roberts (1980)

$$\mathrm{sign}(A) = A \left(\sqrt[2]{A^2} \right)^{-1}$$

principal *p*th root

Padé iterations

- sign function
  Kenney, Laub (1991)

- square root
  Higham, Mackey, Mackey, Tisseur (2004)

- p-sector function and pth root
  Laszkiewicz, Zietak (2009)

Padé family of iterations for matrix sector function

$$\mathrm{sect}_p(\lambda) = \frac{\lambda}{\sqrt[p]{\lambda^p}} = \frac{\lambda}{\sqrt[p]{1-z}}$$

$$z = 1 - \lambda^p$$

$$X_{j+1} = X_j R_{km}(I - X_j^p), \qquad X_0 = A$$

$R_{km}(z)$ is
$[k/m]$ Padé approximant to $\quad f(z) = \frac{1}{\sqrt[p]{1-z}}$

Structure-preserving rational matrix iterations

structure-preserving

$$X_{k+1} = h(X_k) \in \mathbb{G} \quad \text{if} \quad X_0 = A \in \mathbb{G}$$

$\mathbb{G}$ automorphism group - Higham, Mackey, Tisseur 2004

If

$$h(x) = x^r \frac{a_0 + a_1 x^t + a_2 x^{2t} + \cdots + a_k x^{kt}}{a_k + a_{k-1} x^t + a_{k-2} x^{2t} + \cdots + a_0 x^{kt}}$$

then structure-preserving in $\mathbb{G}$.

Automorphism groups $\mathbb{G}$

$$A^\star = M^{-1}A^TM, \quad \text{or} \quad A^\star = M^{-1}A^*M, \quad \textbf{adjoint}$$

$$\mathbb{G} = \{A : A^\star = A^{-1}\}$$

bilinear (real or complex) or sesquilinear forms

$$< x, y >= x^TMy, \quad < x, y >= x^*My$$

Examples of automorphism groups

- $M = I$, A real, $\mathbb{G}$ – real orthogonals
- $M = I$, A complex, $\mathbb{G}$ – unitaries
- $M = I$, A complex, $\mathbb{G}$ – complex orthogonals
- $M = J$, A real, $\mathbb{G}$ – real sympletics
- sympletics, perpletics, pseudo-unitaries,...

Structure-preserving iterations in automorphism groups:

- Higham Mackey, Tisseur (2004) – principal Padé iterations for matrix sign
- Iannazzo (2008)– some methods from König's family of iterations for matrix sector
- Laszkiewicz-Ziętak (2009) – principal Padé iterations for matrix sector

Principal Padé iterations for sector

$$h_{mm}(x) = x\frac{\sum_{j=0}^{m} b_j^{(m)} x^{pj}}{\sum_{j=0}^{m} c_j^{(m)} x^{pj}}$$

$$b_j^{(m)} = (-1)^j \sum_{k=j}^{m} \binom{k}{j} \frac{\left(\frac{1}{p}\right)_k (\frac{1}{p} - m)_m (k-2m)_m}{k!(-2m)_m (k+\frac{1}{p}-m)_m}$$

$$(\alpha)_j = \alpha(\alpha+1)\dots(\alpha+j-1)$$

by means of Zeilberger algorithm

$$b_j^{(m)} = \binom{m}{j} \frac{m!}{(2m)!p^m} \prod_{k=m-j+1} (kp-1) \prod_{k=j+1} (kp+1),$$

Pure matrix iterations, Iannazzo (2008)

$$X_{k+1} = h(X_k), \qquad X_0 = X_0(A)$$

$h(X)$ does not depend on A

Corollary

If scalar Padé iterations converge to $\mathrm{sect}_p(\lambda_j)$ for every eigenvalue $\lambda_j(A)$ then matrix Padé iterations are convergent to $\mathrm{sect}_p(A)$.

Regions of convergence for p-sector

$\mathbf{p = 5}$

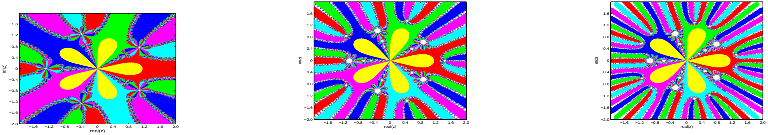


Figure: [0/1], [0/2], [0/3]

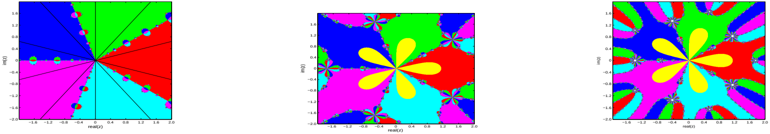


Figure: [1/1], [1/2], [1/3]

$[k/m]$ Padé iterations **for sign** $(p = 2)$

Kenney, Laub (1991) - local convergence for $k > m - 1$

If

$$|1 - z_0^2| < 1$$

then

$$|1 - z_j^2| \leq |1 - z_0^2|^{(k+m+1)^j}$$

$$\lim_{j \to \infty} z_j = sign(z_0)$$

Global convergence for sign, $[m/m]$, $[m-1/m]$

Goal:

conjecture of Laszkiewicz and Zię̦tak (2009)

Convergence of all $[k/m]$ Padé iterations to p-sector for z_0 in

$$\{z \in \mathbb{C} : \; |1 - z^p| < 1\}$$

Conjecture has been proved

- by Gomilko, Greco, Ziętak for sign (2011)
- by Gomilko, Karp, Lin, Ziętak for sector (2012)

Speed of convergence for "sector" (Gomilko,Karp,Lin,Zięṭak)

If $|1 - z_0^p| < 1$ then

$$|1 - z_\ell^p| \leq |1 - z_0^p|^{(k+m+1)^\ell} M$$

where

$$M = \left(\frac{|1 - z_0^p| + \alpha}{\alpha |1 - z_0^p| + 1} \right)^{((k+m+1)^\ell - 1)/(k+m)}$$

$$\alpha = \alpha(p, k, m) < 1$$

[1/1] Halley, $\alpha = \frac{(p^2-1)}{12p^2}$

- **Properties of Padé approximants to** $(1-z)^{-1/p}$
- Localization of **roots** of certain polynomials (**denominators of Padé approximants**)
- Identities involving **hypergeometric functions**
- Signs of coefficients of **reciprocals of some power series and polynomials**

Crucial function

$$1 - (1 - z)\left(\frac{P_{km}(z)}{Q_{km}(z)}\right)^p$$

show: all Taylor coefficients are positive !!!

$$\frac{P_{km}(z)}{Q_{km}(z)} \quad \textit{is} \quad [k/m] \text{ Pade approximant}$$

to

$$\frac{1}{(1 - z)^{1/p}}$$

Comparison of two cases of $[k/m]$ for **sign** $k \geq m-1$ and $k < m-1$

$$1-(1-z)\left(\frac{P_{km}(z)}{Q_{km}(z)}\right)^2 = \frac{Q_{km}^2(z)-(1-z)P_{km}^2(z)}{Q_{km}^2(z)}$$

for the both cases all coefficients of polynomial
$Q_{km}^2 - (1-z)P_{km}^2$ are positive
and $|Q_{km}(z)| > Q_{km}(1), \qquad |z| < 1$

for $k \geq m-1$ all roots of Q_{km} lay in $(1,\infty)$ (**Kenney-Laub**)

for $k < m-1$ there are some (complex) roots outside of $(1,\infty)$ (**Gomilko-Greco-Ziętak**)

$$f(z) = \frac{1}{(1-z)^{1/p}} = {}_2F_1\left(\frac{1}{p}, 1; 1; z\right)$$

${}_2F_1$ Gauss hypergeometric function

$$\operatorname{sect}_p(\lambda) = \frac{\lambda}{\sqrt[p]{\lambda^p}}$$

$$= \frac{\lambda}{\sqrt[p]{1-(1-\lambda^p)}} = \lambda f(1-\lambda^p)$$

Gauss hypergeometric functions - notation

$$ {}_2F_1(\alpha, \beta; \gamma; z) = \sum_{j=0}^{\infty} \frac{(\alpha)_j (\beta)_j}{j!(\gamma)_j} z^j, \quad |z| < 1 $$

Pochhammer's symbol
$(\alpha)_j = \alpha(\alpha+1)\cdots(\alpha+j-1), \quad (\alpha)_0 = 1.$

$[k/m]$ Padé approximant to $(1-z)^{-1/p}$

$k \geq m-1$, Wimp, Beckermann (1993)
k, m arbitrary, Gomilko, Greco, Zietak (2011)

$$R_{km}(z) = \frac{P_{km}(z)}{Q_{km}(z)}$$

where

$$Q_{km}(z) = {}_2F_1\left(-m, -\frac{1}{p} - k; -k-m; z\right)$$

$$P_{km}(z) = {}_2F_1\left(-k, \frac{1}{p} - m; -k-m; z\right)$$

Properties of $[k/m]$ Padé approximants

$$(\mathbf{1}-\mathbf{z})^{-\sigma}, \qquad \mathbf{0}<\sigma<\mathbf{1}$$

Kenney, Laub (1991)

If $k \geq m-1$ then all poles are bigger than 1.

Gomilko, Greco, Ziętak (2011)

If $k < m-1$ then

- $k+1$ poles are bigger than 1
- the remaining poles have moduli bigger than 1

Roots of polynomials $w(x) = a_n x^n + a_{n-1} x^{n-1} + \cdots + a_0$

- **Kakeya**: If $0 < a_n < a_{n-1} < \cdots < a_0$ then roots $|r_j| > 1$
- **GGZ (2011)**:
  If $a_0 > 0$,
  $\mathrm{sign}(a_j) = (-1)^{k+1}$ for $j = k+2, \ldots, n$
  $w(x)$ has $k+1$ roots bigger than 1
  then
    - remaining roots have moduli bigger than 1
    - all coefficients of power series expansion of reciprocal $\frac{1}{w(x)}$ are positive

Padé approximants to Stieltjes functions

Baker, Graves-Morris

Let $F(z)$ be a Sieltjes function. Then for $k \geq m-1$ the $[k/m]$ **Padé approximant** to $F(z)$ has the power series expansion with all coefficients positive.

Gomilko, Karp, Lin, Ziętak

Every $[k/m]$ **Padé approximant** to $(1-z)^{-\sigma}$, $0 < \sigma < 1$, has the power series expansion with all coefficients positive.

Stieltjes functions

$$F(z) = \sum_{j=0}^{\infty} d_j (-z)^j = \int_0^{\infty} \frac{d\varphi(u)}{1+zu},$$

$$\varphi(u) \; bounded, \;\; nondecreasing$$

$$\int_0^{\infty} u^j d\varphi(u), \quad finite \;\; moments$$

$$(j = 0, 1, 2, \ldots)$$

Reciprocal of some power series

Gomilko, Greco, Ziętak 2011

Let analytical function

$$F(z) = \sum_{j=0}^{\infty} d_j z^j, \qquad F(0) > 0$$

have $r_1, \ldots, r_k$ roots in $(0, \gamma)$,

$$(-1)^{k+1} d_j \geq 0, \quad j \geq k+1.$$

Then all coefficients of the power series expansion of the reciprocal of $F(z)$ are positive.

investigations initiated by Kaluza in 1928

Identities for $(1-z)^{-\sigma}, \qquad 0 < \sigma < 1$

$$(1-z)^{-\sigma} - [k/m] = Dz^{k+m+1}\frac{S_{km}(z)}{Q_{km}(z)}$$

$$[k+1/m+1] - [k/m] = Dz^{k+m+1}\frac{1}{Q_{k+1,m+1}(z)Q_{k,m}(z)}$$

$$D > 0$$

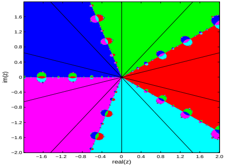
Conjecture for p-sector (Laszkiewicz, Zietak 2009)

If

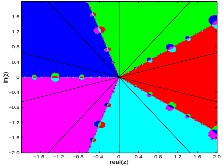
$$z_0 \in \bigcup_{k=0}^{p-1} \left\{ z \in \mathbb{C} : \frac{2k\pi}{p} - \frac{\pi}{2p} < \arg(z) < \frac{2k\pi}{p} + \frac{\pi}{2p} \right\}$$

then $[k/k]$ Padé iteration is convergent.

$[1/1]$ Halley–true



$[2/2]$



Greco, Iannazzo, Poloni (2012)

reciprocal (dual) Padé iterations for sign

Pade iterations and its reciprocals for sign

Greco-Iannazzo-Poloni (2012)

$$z_{\ell+1} = \frac{Q_{km}(1 - z_\ell^2)}{z_\ell P_{km}(1 - z_\ell^2)}, \qquad z_0 = z$$

Kenney-Laub (1991)

$$z_{\ell+1} = \frac{z_\ell P_{km}(1 - z_\ell^2)}{Q_{km}(1 - z_\ell^2)}, \qquad z_0 = z$$

$P_{km}(\xi)/Q_{km}(\xi)$ is $[k/m]$ Padé approximant to the function $(1-\xi)^{-1/2}$.

References

- **Greco, Iannazzo, Poloni**, *The Padé iterations for the matrix sign function and their reciprocal are optimal*, `Lin. Alg. Appl.` 436 (2012).
- **Higham, Mackey, Tisseur**, *Computing the polar decomposition and the matrix sign decomposition in matrix groups*, `SIAM J. Matrix Anal. Appl.` 25 (2004).
- **Iannazzo**, *A family of rational iteration and its applications to the computation of the matrix pth root*, `SIAM J. Matrix Anal. Appl.` 30 (2008).
- **Kenney, Laub**, *Rational iterative methods for the matrix sign function*, `SIAM J. Matrix Anal. Appl.` 12 (1991).

THANK YOU!!!

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