Padé approximants of $(1-z)^{-1/p}$ and their applications to computing the matrix p-sector function and the matrix pth roots

Krystyna Ziętak

March 17, 2015

Outline

The talk is based on:

- **Gomilko, Greco, Ziętak,** A Padé family of iterations for the matrix sign function and related problems, *Numer. Lin. Alg. Appl.* (2012).
- **Gomilko, Karp, Lin, Ziętak,** Regions of convergence of a Padé family of iterations for the matrix sector function, *J. Comput. Appl. Math.* (2012).
- **Laszkiewicz, Ziętak,** A Padé family of iterations for the matrix sector function and the matrix pth root, *Numer. Lin. Alg. Appl.* (2009).
- **Ziętak**, The dual Padé families of iterations for the matrix pth root and the matrix p-sector function, *J. Comput. Appl. Math.* (2014).

Coauthors

- Oleksandr Gomilko
  (Toruń, Poland, and Kiev, Ukraine)
- Federico Greco (Perugia, Italy)
- Dmitry B. Karp (Vladivostok, Russia)
- Beata Laszkiewicz (Jelenia Gora, Poland)
- Minghua Lin (Waterloo, Canada)

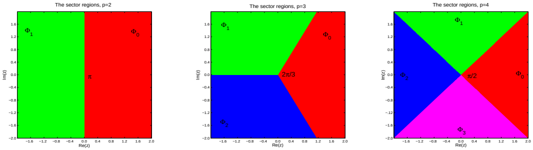
scalar p-sector function, $z \in \mathbb{C}$

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

the nearest *pth* root of unity to z

for $p = 2$ sign function

$$\mathrm{sign}(z) = \begin{cases} 1 & \text{if } \mathrm{Re}(z) > 0 \\ -1 & \text{if } \mathrm{Re}(z) < 0 \end{cases}$$



red - principal sector Φ_0

matrix p-sector function

A nonsingular

$$\mathrm{sect}_p(A) = A(A^p)^{-1/p}$$

$$\arg(\lambda_j(A)) \neq (2q+1)\pi/p, \qquad q = 0, 1, \ldots, p-1$$

matrix principal pth root $X = A^{1/p}$

$$X^p = A, \qquad \lambda_j(X) \in \Phi_0$$

no eigenvalue of A lies on closed negative real axis

Canonical Jordan form

$$A = WJW^{-1}$$

Matrix *p*-sector function

$$\mathrm{sect}_p(A) = W \, \mathrm{diag}\left(sect_p(\lambda_j)\right) \, W^{-1}$$

λ_j eigenvalues of A

applications of $sign(A)$

- solving the matrix equations of Sylvester, Lyapunov, Riccati,
- p - number of eigenvalues of A of order n in the open left half-plane,
  q - number of eigenvalues in the open right half-plane

$$p = \frac{1}{2}(n - \mathrm{trace}(\mathrm{sign}(A)), \quad q = \frac{1}{2}(n + \mathrm{trace}(\mathrm{sign}(A))$$

- quantum chromodynamics, lattice QCD, the overlap-Dirac operator of Neuberger – solving the linear systems

$$(G - \mathrm{sign}(H))x = b$$

see, for example, N.J.Higham, *Functions of Matrices. Theory and Computation*, SIAM 2008.

Applications of matrix p-sector function

- determining the number of eigenvalues in a specific sector
- obtaining corresponding invariant subspaces

After suitable change of variable, iterations for computing $\mathrm{sect}_p(A)$ can be applied to computing

- pth roots of a matrix
- polar decomposition of a matrix ($p = 2$)

$[k/m]$ Pade approximant to $g(z)$

$$g(z) - \frac{P_{km}(z)}{Q_{km}(z)} = O(z^{k+m+1})$$

$P_{km}(z)$ polynomial of degree $\leq k$
$Q_{km}(z)$ polynomial of degree $\leq m$

$$g(z) = (1 - z)^{-1/p} = {}_2F_1(1/p, 1; 1; z)$$

Gauss hypergeometric function

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

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

Padé approximants to $(1-z)^{-1/p}$

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

Gomilko, Greco, KZI (2012)

formula for denominators of Padé approximants of ${}_2F_1(a, 1; c; z)$, $k \geq m-1$:

- H. van Rossum (1955)
- Baker, Graves-Morris - books (1975, 1981)
- Kenney, Laub (1989, 1991)
- Wimp, Beckermann (1993)

Padé approximants

$$(1-z)^{-\sigma}, \quad \sigma \in (0,1)$$

Numerators

- Kenney and Laub (1991), $\quad p = 2$

$$P_{km}(z) = \sum_{j=0}^{k} \frac{(\dots)}{(\dots)} z^j$$

- Driver, Jordaan (2002, 2009)

$$P_{km}(z) = \sum_{j=0}^{k} \sum_{i=0}^{j} \frac{(\dots)}{(\dots)} z^j$$

$0 < \sigma < 1$

- $[k/m]$ Padé approximant to $(1-z)^{-\sigma}$ is the reciprocal of $[m/k]$ approximant to $(1-z)^{\sigma}$.
- $P_{km}(1) < |P_{km}(z)|$ for $|z| < 1$.
- $Q_{km}(1) < |Q_{km}(z)|$ for $|z| < 1$.
- $$\frac{Q_{kk}(1)}{P_{kk}(1)} = \frac{(-\sigma+1)_k}{(\sigma+1)_k} < 1$$

Padé approximants

$$(1-z)^{-\sigma}, \quad \sigma \in (0,1)$$

Error (GKLZ 2012)

$$\frac{P_{km}(z)}{Q_{km}(z)} = (1-z)^{-\sigma} - D_{km}^{(\sigma)} z^{k+m+1} \, \frac{{}_2F_1(\dots)}{Q_{km}(z)}$$

$$D_{km}^{(\sigma)} > 0, \quad \text{constant, given explicitly}$$

Laszkiewicz, KZI 2009

$$P_{kk}(1 - z^p) = \mathrm{rev}(Q_{kk}(1 - z^p))$$

$$\mathrm{rev}\left(a_0 z^k + a_1 z^{k-1} + \ldots + a_k\right) = a_k z^k + a_{k-1} z^{k-1} + \ldots + a_0$$

proof - Zeilberger algorithm

- structure preserving (in automorphism groups) by Padé iterations for p-sector function
- construction of generally convergent iterative methods for roots of polynomial $z^3 - 1$

Hawkins (2002) gives two generally convergent methods for $z^3 - 1$, which in fact are generated by principal Padé iterations for sector ($p = 3$).

$$P_{mm}(1-z^p) = \sum_{j=0}^{m} b_j z^j$$

$$b_j = (-1)^j \frac{(1/p-m)_m}{(-2m)_m} \sum_{\ell=j}^{m} \binom{\ell}{j} \frac{(1/p)_\ell (\ell-2m)_m}{\ell!(\ell+1/p-m)_m}$$

$$= \binom{m}{j} \frac{m!}{(2m)!p^m} \prod_{\ell=m-j+1}^{m} (\ell p - 1) \prod_{\ell=j+1}^{m} (\ell p + 1)$$

auxiliary function $F(j) = \sum \ldots$

$$F(j) + (1-p(j+1))F(j+1) = 0, \quad F(j) = \prod_{\ell=j+1}^{m} (\ell p - 1)$$

proof - Zeilberger algorithm

Roots and poles of $[k/m]$ Padé approximants

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

Kenney, Laub (1991)

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

Gomilko, Greco, KZI (2011)

- If $k < m - 1$, then $k + 1$ poles are bigger than 1, the remaining poles have moduli bigger than 1.
- If $1 \leq k \leq m$, then all roots of $P_{km}(z)$ lie in $(1, \infty)$
- If $k > m \geq 1$, then m roots of $P_{km}(z)$ lie in $(1, \infty)$, remaining roots have moduli bigger than 1

K. Driver and K. Jordaan (2002, 2008)

Zeros of polynomials ${}_2F_1(-n, b; c; z)$

- For $c > 0$ and $b > +n - 1$, all zeros are simple and lie in $(0, 1)$
- For $b < 1 - n$ and $d > 0$, all zeros are simple and lie in $(-\infty, 0)$
- ...
- For $-n < b < 0$, if

$$-k < b < -k + 1,$$

for some $k \in \{1, \dots, n\}$, then

  - k zeros in $(1, \infty)$,
  - In addition, if $(n - k)$ is even, then $(n - k)$ zeros is non-real; if $(n - k)$ is odd, then one real negative zero and $(n - k - 1)$ zeros is non-real.

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 satisfy $|r_j| > 1$.
- **Gomilko, Greco, KZI (2011)**: Let
  - $a_0 > 0$,
  - $\mathrm{sign}(a_j) = (-1)^{k+1}$ for $j = k+2, \ldots, n$,
  - $w(x)$ has $k+1$ roots bigger than 1.

  Then remaining roots have moduli bigger than 1.

Crucial function

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

show: all Taylor coefficients are positive !!!

Remark. This function is applied in the proof of local convergence of some iterative methods for $\mathrm{sect}_p(A)$.

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

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

Comparison: cases $k \geq m-1$ and $k < m-1$ for $p = 2$

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

for the both cases all coefficients of polynomial $Q_{km}^2 - (1-z)P_{km}^2$ are positive

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

for $k < m-1$ there are some roots of Q_{km} outside of $(1, \infty)$

$$|Q_{km}(z)| > Q_{km}(1), \qquad |z| < 1$$

$r_j > 0$ for $j = 1, \ldots, k$ roots of polynomial $u(z)$ of order n

Power series expansion of $1/u(z)$

$$u(z) = r_1 r_2 \cdots r_k \left(1 - \frac{z}{r_1}\right) \cdots \left(1 - \frac{z}{r_k}\right) v(z)$$

$$\frac{1}{1-z} = 1 + z + z^2 + \cdots$$

$$u(z) = Q_{km}(z)$$

Reciprocal of some power series

Gomilko, Greco, KZI 2011

Let

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

be analytical in $|z| < \gamma$ and let $F(z)$ have roots $r_1, \ldots, r_k$ counted with multiplicity 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 signs of coefficients of reciprocals of some power series initiated by Kaluza in 1928

Theorem of Kaluza (1928)

Let

$$\frac{1}{1+\sum_{k=1}^{\infty} a_k z^k} = 1 - \sum_{k=1}^{\infty} b_k z^k.$$

If $a_k > 0$ and

$$a_k^2 \le a_{k-1} a_{k+1},$$

then $0 \le b_k \le a_k$.

Coefficients of power series expansions are positive

(Gomilko, Greco, KZI, 2012)

$$\frac{1}{Q_{km}(z)}$$

denominator of Padé approximant of $(1-z)^{-\sigma}$

Gomilko, Karp, Lin, KZI (2012)

- $[k/m]$ Padé approximant to $(1-z)^{-\sigma}$
- $$f_{km}(z) = 1 - (1-z)\left(\frac{P_{km}(z)}{Q_{km}(z)}\right)^p$$

Padé approximants to Stieltjes functions

Baker, Graves-Morris

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

Remark. ${}_2F_1(1, b; c; -z)$ is Stieltjes for $c > b > 0$. Thus we can apply the theorem to $(1+z)^{-\sigma} = (1-(-z))^{-\sigma} = g(-z)$.

Stieltjes functions

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

$$\varphi(u) \ \textit{bounded}, \ \textit{nondecreasing}$$

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

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

Hypergeometric functions ${}_2\mathbf{F}_1(-\mathbf{m}, \mathbf{b}; -\mathbf{n}; \mathbf{z})$

- Luke, book 1969
  $\mathbf{n} < \mathbf{m}$ - not defined; $\mathbf{m} = \mathbf{n}$, $(1-z)^{-b}$
  for $\mathbf{n} > \mathbf{m}$

$$ {}_2F_1(-m, b; -n; z) = \sum_{j=0}^{m} \frac{(-m)_j (b)_j z^j}{j!(-n)_j} + \sum_{j=n+1}^{\infty} \frac{(-m)_j (b)_j z^j}{j!(-n)_j} $$

- Bateman, Erdelyi (1953), Temme 1996
  $\mathbf{n} = \mathbf{m}$,

$$ {}_2F_1(-m, b; -m; z) = \sum_{j=0}^{m} \frac{(b)_j z^j}{j!} $$

for $\mathbf{n} = \mathbf{m} + \mathbf{q}$, $\mathbf{q} = 1, 2, \ldots$

$$ {}_2F_1(-m, b; -m-q; z) = \sum_{j=0}^{m} \frac{(-m)_j (b)_j z^j}{(-m-q)_j} $$

Clausen formula

$$\left({}_2F_1(a,b;a+b+\frac{1}{2};z)\right)^2 = {}_3F_2(2a,2b,a{+}b;2a{+}2b,a{+}b{+}\frac{1}{2};z)$$

hypergeometric polynomials, for $k < m-1$ Gomilko, Greco, KZI 2012

$$a=-m, \quad b=-\frac{1}{2}-k$$

$$\left({}_2F_1(-m,-\frac{1}{2}-k;-k-m;z)\right)^2 = \sum_{j=0}^{k+m}\ldots + \sum_{j=k+m+1}^{2m}\ldots$$

$(-r)_s^+ = (-r)(-r+1)\ldots(-1)(1)(2)\ldots(-r+s-1) = (-1)^r r!(s-r-1)!$ for $s > r$

Identity - Gomilko, Karp, Lin, KZI (2012)

Let

$H(z) = {}_2F_1(a, b; c; z), \quad G(z) = {}_2F_1(1-a, 1-b; 2-c; z).$

Then

$$[z(a+b-1)-c+1]\,H(z)G(z)+$$
$$z(1-z)\,[H(z)G'(z)-G(z)H'(z)] =$$
$$1-c$$

related to Legendre's identity, Elliott's identity, Anderson-Vamanamurthy-Vuorinen's identity

Elliott's identity

$${}_2F_1(\ldots; r)\,{}_2F_1(\ldots; 1-r) + {}_2F_1(\ldots; r)\,{}_2F_1(\ldots; 1-r) -$$
$${}_2F_1(\ldots; r)\,{}_2F_1(\ldots; 1-r) = \ldots$$

Iterations generated by Padé approximants

- sign function
  Kenney, Laub (1991)
- square root
  Higham (1997)
  Higham, Mackey, Mackey, Tisseur (2004)
- polar decomposition
  Higham, Functions of Matrices,... (2008)
- p-sector function and pth root
  Laszkiewicz, KZI (2009)
- sign function
  reciprocal Padé iterations
  Greco-Iannazzo-Poloni (2012)
- p-sector function and pth root
  dual Padé iterations, *KZI* (2014)

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

$$\mathrm{sect}_p(t) = t(1-z)^{-1/p}$$

$$z = 1 - t^p, \qquad t^p = 1 - z$$

$\frac{P_{km}(z)}{Q_{km}(z)}$ - Padé approximant of $g(z) = (1-z)^{-1/p}$

$$\mathrm{sect}_p(t) \approx t\frac{P_{km}(1-t^p)}{Q_{km}(1-t^p)}$$

Iterations for matrix p-sector function

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

Laszkiewicz, KZI (2009)

for $p = 2$ (sign) *Kenney-Laub (1991)*

Halley $k = m = 1$

dual Pade $$X_{j+1} = X_j \frac{Q_{km}(I - X_j^{-p})}{P_{km}(I - X_j^{-p})}, \qquad X_0 = A$$

KZI (2014)

Halley $k = m = 1$, Newton $k = 0, m = 1$

Schröder $k = 0$, m arbitrary *Cardoso, Loureiro (2011)*

Principal Padé iterations ($k = m$) for p-sector are **structure preserving** in automorphism groups of matrices.

arbitrary p - Laszkiewicz, KZI (2009)
$p = 2$ Higham, Mackey, Mackey, Tisseur (2004)

automorphism groups: unitaries, sympletics, perpletics,...

defined by bilinear and sequilinear forms

$$\langle Ax, Ay \rangle = < x, y >$$

After suitable change of variable, (dual) Padé iterations for p-sector can be applied to computing

- pth roots
- square root ($p = 2$)
- polar decomposition

Convergence of pure matrix iterations (Iannazzo, 2008)

convergence of scalar sequences of eigenvalues $\rightarrow$ convergence of matrix sequences

(dual) Padé iterations for p-sector are pure matrix iterations

Certain regions of convergence for p-sector function

eigenvalues $\lambda_j(A)$ in regions:

Padé iterations - Gomilko, Karp, Lin, KZI 2012

$$\mathbb{L}_p = \{z \in \mathbb{C} : |1 - z^p| < 1\}, \quad X_0 = A$$

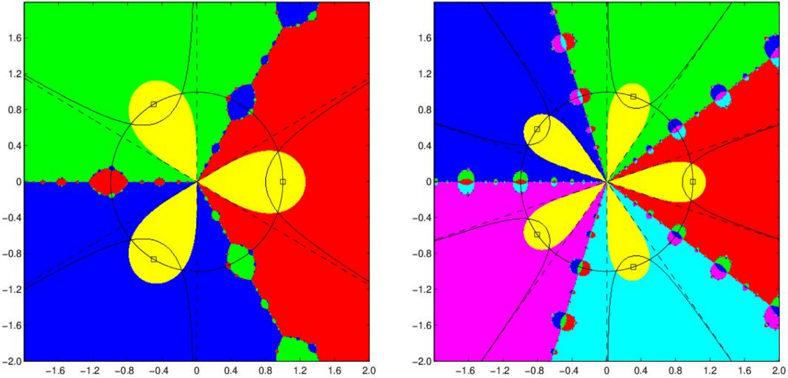
"yellow flowers" - it was conjectured by Laszkiewicz, KZI 2009

dual _Padé_ iterations - KZI 2014

$$\mathbb{L}_{-p} = \{z \in \mathbb{C} : |1 - z^{-p}| < 1\}, \quad X_0 = A$$

solid countur

In th proof one applies that coefficients of the power series expansion of $f_{km}(z) = 1 - (1 - z)\left(\frac{P_{km}(z)}{Q_{km}(z)}\right)^p$ are positive



Halley iterations for $p = 3$ and $p = 5$
the unit circle (solid contour), the pth roots of unity (boxes)
$\mathbb{L}_p^{(Pade)}$ for "Padé" (yellow flower)
$\mathbb{L}_{-p}^{(Pade)}$ for "dual Padé" (solid contour)

Padé approximant to $g(z) = (1-z)^{-1/2}$,
notation $1/Q_{km}(X) = (Q_{km}(X))^{-1}$

Padé for sign (Kenney-Laub, 1991)

$$Y_{j+1} = Y_j \frac{P_{km}(I - Y_j^2)}{Q_{km}(I - Y_j^2)}, \qquad Y_0 = A$$

reciprocal Padé for sign (Greco-Iannazzo-Poloni, 2012)

$$Y_{j+1} = \frac{Q_{km}(I - Y_j^2)}{Y_j P_{km}(I - Y_j^2)}, \qquad Y_0 = A$$

dual Padé for sign (KZI 2014)

$$Y_{j+1} = \frac{Y_j Q_{km}(I - Y_j^{-2})}{P_{km}(I - Y_j^{-2})}, \qquad Y_0 = A$$

Computing $A^{1/p}$, Laszkiewicz, KZI 2009

Padé iterations

$$X_{i+1} = X_i P_{km}(I - A^{-1}X_i^p)\left(Q_{km}(I - A^{-1}X_i^p)\right)^{-1}, \quad X_0 = I$$

$A^{1/p}$, coupled stable Padé iterations (Laszkiewicz, KZI 2009)

$$X_{i+1} = X_i h(Y_i), \quad Y_{i+1} = Y_i(h(Y_i))^p, \quad X_0 = I, Y_0 = A^{-1}$$

where $h(t) = P_{km}(1 - t)/Q_{km}(1 - t)$

Computing $A^{1/p}$, KZI 2014

Dual Padé iterations

$$X_{i+1} = X_i P_{km}(I - AX_i^{-p})\left(Q_{km}(I - AX_i^{-p})\right)^{-1}, \quad X_0 = I$$

Properties of dual Padé family for pth root

KZI 2014

residuals for Padé iteration generated by $[k/m]$

$$S_\ell = I - A^{-1}X_\ell^p$$

$$S_{\ell+1} = f_{km}(S_\ell)$$

residuals for dual Padé iteration generated by $[k/m]$

$$R_\ell = I - AX_\ell^{-p}$$

$$R_{\ell+1} = f_{km}(R_\ell)$$

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

Guo (2010) applies "dual residuals" to investigation of convergence of Newton and Halley iterations

binomial expansion

$$(1-z)^{1/p} = \sum_{j=0}^{\infty} \beta_j z^j$$

KZI 2014

the ℓth iterate Y_ℓ, computed by the dual Padé iteration generated by $[k/m]$ Padé approximant applied to computing $(I-B)^{1/p}$, satisfies

$$Y_\ell = \sum_{j=0}^{\infty} \varphi_{km,j}^{(\ell)} B^j$$

where $\varphi_{km,j}^{(\ell)} = \beta_j$ for $j = 0, \ldots, (k+m+1)^\ell - 1$

Guo (2010) - Newton ($k=0, m=1$) and Halley ($k=m=1$)
KZI (2014) - arbitrary k, m

References I

- **Cardoso, Loureiro**, On the convergence of Schröder iteration functions for pth roots of complex numbers, *Appl. Math. Comput.* 217 (2011).
- **Greco, Iannazzo, Poloni**, The Padé iterations for the matrix sign function and their reciprocal are optimal, *Lin. Alg. Appl.* (2012).
- **Guo**, On Newton's and Halley's method for the principal pth root of a matrix, *Lin. Alg. Appl.* (2010).
- **Higham, Mackey, Mackey, Tisseur**, Computing the polar decomposition and the matrix sign decomposition in matrix group, *SIAM J. Matrix Anal.* 25 (2004).
- **Kenney, Laub**, Rational iterative methods for the matrix sign function, *SIAM J. Matrix Anal. Appl.* 12 (1991).

Reference II

- **Anderson, Staff, Varga**, On the Eneström-Kakeya theorem and its sharpness, *Linear Alg. Appl*. (1997).
- **Driver, Jordaan**, Convergence of ray sequences of Padé approximants for ${}_2F_1(a, 1; c; z), (c > a)$, Questiones Mathematicae 25 (2002). c and cubic transformation
- **Driver, Jordaan**, Zeros of the hypergeometric polynomial $F(-n, b; c; z)$, Algorithms for Approx. IV (2002); arXiv 0812.0708v1 (2008).
- **Kaluza**, Über die Koeffizienten reziproker Potenzreihen, *Mathematische Zeitschrif* 28 (1928).
- **Wimp, Beckermann**, Some explicit formulas for Padé approximants of ratios of hypergeometric functions, *WSSIAA* 2 (1992).

Reference III

- **Roberts**, Linear model reduction and solution of the algebraic Riccati equation by use of the sign function, *Internat. J. Control* 32 (1980).
- **Shieh, Tsay, Wang**, Matrix sector functions and their applications to system theory, *Proc. IEE Control Theory and Appl.* 131 (1984).