Journal of Computational and Applied Mathematics 236 (2012) 4410–4420

Contents lists available at SciVerse ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

Regions of convergence of a Padé family of iterations for the matrix sector function and the matrix pth root

Oleksandr Gomilko [a], Dmitry B. Karp [b], Minghua Lin [c,1], Krystyna Ziętak [d,*]

[a] Faculty of Mathematics and Computer Science, Nicolas Copernicus University, 87-100 Toruń, Poland
[b] School of Economics and Management, Far Eastern Federal University, 690950 Vladivostok, Okeanskii Prospekt 19, Russian Federation
[c] Department of Mathematics and Statistics, University of Regina, Regina, S4S 0A2, Canada
[d] Institute of Mathematics and Computer Science, Wrocław University of Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland

ARTICLE INFO

Article history:
Received 18 April 2011
Received in revised form 17 January 2012

MSC:
33F05
65D20

Keywords:
Matrix sector function
Matrix root
Rational matrix iteration
Padé approximant
Hypergeometric function
Hypergeometric identity

ABSTRACT

In this paper, we prove a conjecture on a common region of a convergence of Padé iterations for the matrix sector function. For this purpose, we show that all Padé approximants to a special case of hypergeometric function have a power series expansion with positive coefficients. Using a sharpened version of Schwarz's lemma, we also demonstrate a better estimate of the convergence speed. Our results are also applicable to a family of rational iterations for computing the matrix pth root.

1. Introduction

Algorithms for computing matrix functions are a subject of current research (see, for example, [1]). In this paper, we investigate a convergence of the Padé family of iterations for computing the matrix p-sector function, proposed in [2], which includes the Halley method and the inverse Newton method. These rational iterations can be adapted for computing the matrix pth root. Computation of matrix pth root has recently aroused considerable interest; see, for example, [3–11].

Let $p \geq 2$ be an integer and let z be a non-zero complex number, having the argument $\varphi \in [0, 2\pi)$ different from $(2\ell+1)\pi/p,\ \ell = 0, \ldots, p-1$. Then the scalar p-sector function of z is equal to (see [12])

$$s_p(z) = z(z^p)^{-1/p},$$

where $(z)^{1/p}$ denotes the principal pth root of z. For $p = 2$ the sector function reduces to the sign function. Let $\varepsilon_j = e^{i2\pi j/p}$, $j \in \{0, 1, \ldots, p-1\}$, be one of the pth roots of unity. Then $s_p(z) = \varepsilon_q$ where ε_q is the nearest to z pth root of unity.

The matrix p-sector function is an extension of $s_p(z)$ introduced in [12] (for applications see also [13,14]). For a nonsingular matrix $A \in \mathbb{C}^{n\times n}$ having no eigenvalues with arguments $(2\ell+1)\pi/p,\ \ell = 0, \ldots, p-1$, the matrix p-sector

* Corresponding author.
E-mail addresses: alex@gomilko.com (O. Gomilko), dmkrp@yandex.ru (D.B. Karp), mlin87@ymail.com (M. Lin), krystyna.zietak@pwr.wroc.pl (K. Ziętak).

1 Current address: Department of Applied Mathematics, University of Waterloo, Waterloo, N2L 3G1, Canada.

0377-0427/$ – see front matter
doi:10.1016/j.cam.2012.04.007

function can be defined by

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

where we take the principal pth root (see [1] for the properties of the principal matrix root and algorithms for computing it).

In this paper we use the same notation as in [15] for the $[k/m]$ Padé approximants and the Gauss hypergeometric function ${}_2F_1(a, b; c; z)$. In particular, we use the hypergeometric polynomials

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

where $(b)_j = b(b+1)\cdots(b+j-1)$ for $j > 0$ and $(b)_0 = 1$.

Throughout the paper we will assume that the integers k and m satisfy

$$k \geq 0, \ m \geq 0, \quad k+m \geq 1. \tag{1.1}$$

The rational function $R_{km}^{(F)}(z) = P_{km}^{(F)}(z)/Q_{km}^{(F)}(z)$ is said to be a $[k/m]$ Padé approximant to the function $F(z)$ defined by a formal power series, if the numerator $P_{km}^{(F)}(z)$ has degree at most k, the denominator $Q_{km}^{(F)}(z)$ has degree at most m, and $F(z) - R_{km}^{(F)}(z) = O(z^{k+m+1})$ in a neighborhood of $z = 0$. We assume $Q_{km}^{(F)}(0) = 1$. If a $[k/m]$ approximant exists then it is unique. It is usually required that $P_{km}^{(F)}(z)$ and $Q_{km}^{(F)}(z)$ have no common zeros, so that $P_{km}^{(F)}(z)$ and $Q_{km}^{(F)}(z)$ are unique (see, for example, [1, p. 79]).

The sector function $s_p(z)$ can be expressed in the following way

$$s_p(z) = \frac{z}{(1-(1-z^p))^{1/p}} = \frac{z}{(1-\xi)^{1/p}}, \qquad \xi = 1 - z^p. \tag{1.2}$$

Therefore we consider for $\sigma \in (0, 1)$ the function

$$f_\sigma(z) = (1-z)^{-\sigma} = {}_2F_1(\sigma, 1; 1; z) = \sum_{j=0}^{\infty} \frac{(\sigma)_j (1)_j}{j!(1)_j} z^j = \sum_{j=0}^{\infty} \frac{(\sigma)_j}{j!} z^j. \tag{1.3}$$

The $[k/m]$ Padé approximant to $f_\sigma(z)$ is equal to

$$\frac{P_{km}^{(\sigma)}(z)}{Q_{km}^{(\sigma)}(z)} = \frac{{}_2F_1(-k, \sigma-m; -k-m; z)}{{}_2F_1(-m, -\sigma-k; -k-m; z)} \tag{1.4}$$

(see [15, Theorem 4.1] for arbitrary k, m and [16, Theorem 2] for $k \geq m-1$).

The expression (1.2) motivates the introduction of the Padé family of rational iterations for computing $s_p(z)$ (see [2,15]):

$$z_{\ell+1} = z_\ell \frac{P_{km}^{(1/p)}(1-z_\ell^p)}{Q_{km}^{(1/p)}(1-z_\ell^p)}, \qquad z_0 = z. \tag{1.5}$$

After a suitable change of a variable we obtain the Padé family of iterations for computing the pth root $a^{1/p}$ (see [2, Section 5]):

$$z_{\ell+1} = z_\ell \frac{P_{km}^{(1/p)}\left(1-z_\ell^p/a\right)}{Q_{km}^{(1/p)}\left(1-z_\ell^p/a\right)}, \qquad z_0 = 1. \tag{1.6}$$

For $p = 2$ the iterations (1.5) were proposed in [17] for computing the function $\mathrm{sign}(z)$.

In (1.5) and (1.6) the rational function $P_{km}^{(1/p)}(z)/Q_{km}^{(1/p)}(z)$ is the $[k/m]$ Padé approximant to $(1-z)^{-1/p}$. Examples of the iterations (1.5) for $k, m = 0, 1, 2$ can be found in [2, Table 1].

Scalar iterations (1.5) and (1.6) define the appropriate matrix iterations for computing the matrix p-sector function and the matrix pth root, respectively, by replacing the scalar operations by the matrix operations: multiplication of matrices and matrix inversion. This leads to the Padé family of iterations for computing the matrix p-sector function of A (see [2])

$$Z_{\ell+1} = Z_\ell P_{km}^{(1/p)}(I - Z_\ell^p)\left(Q_{km}^{(1/p)}(I - Z_\ell^p)\right)^{-1}, \qquad Z_0 = A. \tag{1.7}$$

The convergence of the matrix iterations such as those in (1.7) is determined by the convergence of the scalar sequences for the eigenvalues of $Z_0 = A$ (see [9, Theorem 2.4], [2, Corollary 4.1]; see also [7] for a general theory of matrix iterations for computing matrix functions). Thus if for every eigenvalue λ of A the scalar iterations (1.5) with $z_0 = \lambda$ converge to $s_p(\lambda)$, then the matrix iterations (1.7) converge to $\mathrm{sect}_p(A)$. Therefore our goal is to describe the region of convergence for the scalar iterations (1.5). This leads immediately to the regions of convergence of the iterations (1.6) and (1.7).