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The Padé iterations for the matrix sign function and their reciprocals are optimal

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ABSTRACT

It is proved that among the rational iterations locally converging with order $s > 1$ to the sign function, the Padé iterations and their reciprocals are the unique with the lowest sum of the degrees of numerator and denominator.

1. Introduction

The function $s(z) = \text{sign}(z)$ is defined for a nonimaginary complex number z as the nearest square root of unity. Let A be a matrix having no purely imaginary eigenvalues. Since $s(z)$ is analytic at the eigenvalues of A, matrix function theory [5] allows one to define $\text{sign}(A)$. The matrix sign function is less trivial than its scalar counterpart, for instance it is not locally constant, and it has important applications, either direct like the solution of algebraic Riccati equations [12] and the treatment of certain quantum chromodynamics models [19] or indirect as a basis to compute other important matrix functions like the matrix square root, the polar decomposition of a matrix and the geometric mean of two positive definite matrices [5,8].

A common way to compute the matrix sign function is through rational iterations of the form $z_{k+1} = \varphi(z_k)$, for some rational function $\varphi(z)$ having attractive fixed points at 1 and -1, since any

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such iteration converges locally to the function $\operatorname{sign}(z)$. The prototypical example is Newton's method for $z^2 - 1 = 0$, but many other iterations have been proposed. Among them, a very popular family is obtained by using the Padé approximants to $f(\xi) = (1-\xi)^{-1/2}$ and the following characterization

$$\operatorname{sign}(z) = \frac{z}{(z^2)^{1/2}} = \frac{z}{(1-\xi)^{1/2}},$$

where $\xi = 1 - z^2$. Let the (m, n) Padé approximant to $f(\xi)$ be $P_{m,n}(\xi)/Q_{m,n}(\xi)$, and $m + n \geqslant 1$. The iteration

$$z_{k+1} = \frac{z_k P_{m,n}(1-z_k^2)}{Q_{m,n}(1-z_k^2)} =: \varphi_{2m+1,2n} \tag{1}$$

has been proved to be locally convergent to 1 and -1 with order of convergence $m+n+1$ for $m \geqslant n-1$ [10]. The notation $\varphi_{2m+1,2n}$ introduced here highlights the fact that the numerator and denominator of $\varphi_{2m+1,2n}$ have degree $2m+1$ and $2n$, respectively.

We recall that, for integers $m, n \geqslant 0$, the (m, n) Padé approximant to a function $h(z)$ is a rational function $p(z)/q(z)$, where $p(z)$ and $q(z)$ are polynomials of degree m and n, respectively, such that

$$h(z) - \frac{p(z)}{q(z)} = O(z^{m+n+1}).$$

For an introduction to the Padé approximation see the book [1].

The iterations (1) have been derived by Kenney and Laub [10] and are called *Padé family of iterations* or just *Padé iterations*; they have been considered also in [3–5,14,20] for computing matrix functions or invariant subspaces of a matrix. Observe that the definition of Padé iterations in [10] is slightly different from ours, since we exclude the case $m = n = 0$, which yields the trivial iteration $z_{k+1} = \varphi_{1,0}(z_k) = z_k$ being not locally convergent to 1 and -1.

Using the identity

$$\operatorname{sign}(z) = \frac{(z^2)^{1/2}}{z} = \frac{(1-\xi)^{1/2}}{z},$$

and the Padé approximants to $g(\xi) = (1-\xi)^{1/2}$, a different family of iterations having attractive fixed points at 1 and -1 is obtained. If $p(z)/q(z)$ is the (m, n) Padé approximant to the function $h(z)$ and $h(0) \neq 0$, then $q(z)/p(z)$ is the (n, m) approximant to $1/h(z)$ (see [1, Theorem 1.5.1]), thus the (m, n) Padé approximant to $g(\xi)$ is $Q_{n,m}(\xi)/P_{n,m}(\xi)$. The iteration

$$z_{k+1} = \frac{Q_{n,m}(1-z_k^2)}{z_k P_{n,m}(1-z_k^2)} =: \varphi_{2m,2n+1}(z_k) \tag{2}$$

is obtained. We call the iterations (2) *reciprocal Padé iterations* or *reciprocal Padé family*. The possibility to invert the functions defining the Padé iterations is suggested as well by Laub in [15] without further discussions.

Many iterations of interest can be retrieved in the Padé family and its reciprocal: $\varphi_{2,1}$, $\varphi_{3,0}$ and $\varphi_{3,2}$ give Newton's method, the Newton–Schulz iteration and Halley's method for $z^2 - 1 = 0$, respectively. Among the Padé family (1), the most common iterations are those with constant denominator (i.e., $n = 0$ in (1)), and the so-called *principal* Padé iterations, namely, those for which the degrees of the numerator and denominator differ by 1 (i.e., $m = n$ or $m = n - 1$ in (1)). Similarly, the reciprocal Padé family contains iterations with constant numerator ($m = 0$ in (2)) or for which the degrees of the numerator and denominator differ by 1 ($m = n$ or $m = n + 1$ in (2)).

Prior to Kenney and Laub, the Padé iterations for $m = n - 1$ and the reciprocal Padé iterations for $m = n$ have been derived in a different way by Howland [6]; Iannazzo [7] proved that the same iterations obtained by Howland can be retrieved in the family of root-finding algorithms sometimes called König family [2] or basic family [9] and attributed [2] to a paper written by Schröder in 1870 [16,17].

The Padé family and its reciprocal family are just two of the infinite families of rational iterations having the square roots of unity as attractive fixed points. A rationale for their use can be given by their interesting properties (see [5,12] for the case of the Padé family; some analogous properties hold for the reciprocal Padé family). We show that they also have an optimality property: among all rational iterations having order of local convergence $s > 1$ at 1 and -1, they are the unique iterations such that the sum of the degrees of the numerator and denominator is minimal. This is a highly desirable property in terms of computational efficiency: in the *generic* case it is cheaper (in terms of the number of arithmetic operations required) to evaluate $a(z)/b(z)$ than $\tilde{a}(z)/\tilde{b}(z)$ when $\deg(\tilde{a}(z)) + \deg(\tilde{b}(z)) > \deg(a(z)) + \deg(b(z))$ and Horner's scheme is applied.

Let s, m, n be nonnegative integers such that $s > 1$ and $m + n = 2s - 1$. Observe that, letting m, n vary, the family $z_{k+1} = \varphi_{mn}(z_k)$ is the union of the Padé family and its reciprocal family; the parities of m and n distinguish one from the other. The following property of $\varphi_{mn}(z)$ is the main result of the paper and will be proved in the next section.

Theorem 1. *Let $s > 1$ be a nonnegative integer. The functions $\varphi_{mn}(z)$, for $m = 0, 1, \ldots, 2s - 1$ and $n = 2s - m - 1$ define the unique rational iterations of the kind $z_{k+1} = \varphi(z_k)$ such that*

- **O1** *the iteration converges locally to* 1 *and* -1 *with order at least s;*
- **O2** *for every iteration $w_{k+1} = \tilde{\varphi}(w_k) = \tilde{a}(w_k)/\tilde{b}(w_k)$, with $\tilde{a}(z), \tilde{b}(z)$ polynomials, having order at least s in both* 1 *and* -1, *it holds that* $\deg(\tilde{a}(z)) + \deg(\tilde{b}(z)) \geqslant \deg(a(z)) + \deg(b(z))$, *where $a(z)$ and $b(z)$ are coprime polynomials such that $\varphi(z) = a(z)/b(z)$.*

Moreover, the iterations have order exactly s in both 1 *and* -1.

We consider just the case $s > 1$ for two reasons: first, in matrix functions computation, algorithms based on rational iterations are competitive if they converge fast, that is if they are of order at least 2; second, if $s = 1$ a direct computation shows that the unique iterations satisfying **O1** and **O2** are the same as the ones obtained for $s = 2$.

It is worth noting that a rational iteration satisfying **O1** and **O2** for some $s > 1$ is not necessarily the one whose iteration function can be evaluated with the minimal cost. In principle, there can be a special rational function which does not satisfy **O2** and can be evaluated with fewer arithmetic operations. In addition, the same iteration can be evaluated with many different schemes yielding different computational costs, relevant in the matrix case (see [5, Chapter 4]). For the principal Padé iterations, a partial fraction expansion [6,11] and a continued fraction expansion [13] are known and can be used to devise efficient evaluation schemes as in [5, Algorithms 4.9 and 4.10].

For the sake of clarity, we recall some basic definitions regarding iterations of the kind $z_{k+1} = \varphi(z_k)$, where $\varphi(z)$ is a rational function and z_* is a fixed point of $\varphi(z)$, that is, $\varphi(z_*) = z_*$. We say that z_* is an *attractive fixed point* if $|\varphi'(z_*)| < 1$; in that case the iteration is locally convergent to z_*, that is, any initial value z_0 sufficiently close to z_* yields a sequence converging to z_*. We say that the iteration *converges locally to z_* with order $s > 1$* if there exist $M_1, M_2 > 0$ such that for z sufficiently close to z_* it holds that $M_1|z - z_*|^s \leqslant |\varphi(z) - z_*| \leqslant M_2|z - z_*|^s$. Since $\varphi(z)$ is infinitely many differentiable at z_*, this is equivalent to requiring that

$$\varphi(z_*) = z_*, \quad \varphi'(z_*) = \varphi''(z_*) = \cdots = \varphi^{(s-1)}(z_*) = 0, \quad \varphi^{(s)}(z_*) \neq 0. \tag{3}$$

In particular, an iteration having order $s > 1$ at z_* is locally convergent to z_*. Further discussion on this topic can be found in any numerical analysis textbook, for instance [18].

2. Proof of the Theorem 1

The proof of Theorem 1 is given by some Lemmas. We first prove that imposing (3) for a rational function $\varphi(z) = a(z)/b(z)$ is equivalent to imposing some conditions on the polynomials $a(z)$ and $b(z)$ and their derivatives. Then we prove that they can only be satisfied if $\deg(a(z)) + \deg(b(z)) \geqslant 2s - 1$, with equality only for a unique family of polynomials. Finally, we prove that these unique solutions correspond to the Padé family and its reciprocal family.

Lemma 2. *Let $s > 1$ be an integer, $z_{k+1} = \varphi(z_k) = a(z_k)/b(z_k)$ a rational iteration, and z_* be one of its fixed points (in particular, $b(z_*) \neq 0$). The iteration converges locally to z_* with order at least s if and only if*

$$a^{(k)}(z_*) = z_* b^{(k)}(z_*), \quad \text{for } k = 0, 1, \ldots, s-1. \tag{4}$$

If moreover $a^{(s)}(z_*) \neq z_* b^{(s)}(z_*)$ then the order is exactly s.

Proof. The rational iteration converges locally to z_* with order at least s if and only if for z sufficiently close to z_*

$$\varphi(z) - z_* = O((z - z_*)^s). \tag{5}$$

Since $b(z)$ is bounded in a neighborhood of z_*, we may multiply the left-hand side of (5) by $b(z)$ without changing its convergence behavior, thus obtaining

$$a(z) - z_* b(z) = O((z - z_*)^s), \tag{6}$$

which in turn is equivalent to (4). As $b(z_*) \neq 0$, $b(z)$ is bounded away from 0 in a neighborhood of z_*, thus we may divide the left-hand side of (6) by $b(z)$ to reverse the previous step and get (5).

If moreover $a^{(s)}(z_*) \neq z_* b^{(s)}(z_*)$, then (6) does not hold anymore if we replace s with $s+1$, and neither does (5), i.e., the convergence order is exactly s. $\square$

Using conditions (4), we may prove the following bound on the degrees of $a(z)$ and $b(z)$.

Lemma 3. *Let s be a positive integer, and $a(z)$, $b(z)$ two polynomials, not both null, such that*

$$\begin{cases} a^{(k)}(1) = b^{(k)}(1), \\ a^{(k)}(-1) = -b^{(k)}(-1), \end{cases} \quad k = 0, 1, \ldots, s-1. \tag{7}$$

Then $\deg(a(z)) + \deg(b(z)) \geqslant 2s - 1$, with the convention that the degree of the zero polynomial is -1.

Moreover, for each pair (m, n) of integers such that $m + n = 2s - 1$, $\min(m, n) \geqslant -1$, there are two polynomials $a_{mn}(z)$, $b_{mn}(z)$ such that $\deg(a_{mn}(z)) = m$, $\deg(b_{mn}(z)) = n$ and the conditions (7) hold. The polynomials $a_{mn}(z)$ and $b_{mn}(z)$ are unique up to a multiplicative factor, and

$$a_{mn}^{(s)}(1) \neq b_{mn}^{(s)}(1), \qquad a_{mn}^{(s)}(-1) \neq -b_{mn}^{(s)}(-1). \tag{8}$$

Proof. First notice that we may impose without loss of generality that $\deg(a(z)) \geqslant \deg(b(z))$ throughout the proof.

We shall prove the result by induction. For $s = 1$, the result is clear. The conditions that we must meet are $a(1) = b(1)$, $a(-1) = -b(-1)$. Thus $a(z)$ and $b(z)$ cannot be both constant, and the only possibility with $\deg(a(z)) = 1$, $\deg(b(z)) = 0$ is choosing $b(z) = \gamma$, $a(z) = \gamma z$ for some constant $\gamma \neq 0$, while the only possibility with $\deg(a(z)) = 2$, $\deg(b(z)) = -1$ is choosing $b(z) = 0$, $a(z) = \gamma(z-1)(z+1)$ for some constant $\gamma \neq 0$.

Let us suppose that the lemma holds true for a given $\bar{s} - 1$, and prove it for $s = \bar{s}$. Let us take two polynomials $a(z)$, $b(z)$ such that $a^{(k)}(\pm 1) = \pm b^{(k)}(\pm 1)$ for all $k = 1, 2, \ldots, \bar{s} - 1$. If $b(z) \equiv 0$, then $a(z)$ must be a multiple of both $(z-1)^{\bar{s}}$ and $(z+1)^{\bar{s}}$, thus it has degree at least $2\bar{s}$ and the result holds. If $b(z) \neq 0$, we may apply the inductive hypothesis to their derivatives $a^{(1)}(z)$ and $b^{(1)}(z)$, and obtain $\deg(a^{(1)}(z)) + \deg(b^{(1)}(z)) \geqslant 2\bar{s} - 3$. This clearly implies $\deg(a(z)) + \deg(b(z)) \geqslant 2\bar{s} - 1$, since the derivative of a polynomial $p(z)$ has degree $\deg(p(z)) - 1$ (notice that this relation holds also for constant polynomials $p(z) \equiv c \neq 0$, with our choice $\deg(0) = -1$).

Let us turn now to the equality case; we shall prove the uniqueness first, and the existence thereafter, of the two families of polynomials attaining the minimal degrees.

Let m, n be such that $m+n = 2\bar{s}-1$, and $a_{mn}(z)$ and $b_{mn}(z)$ be two polynomials with $\deg(a_{mn}(z)) = m$, $\deg(b_{mn}(z)) = n$ satisfying (7). If $n = -1$, then $a(z)$ must be a polynomial multiple of both $(z-1)^{\bar{s}}$ and $(z+1)^{\bar{s}}$ of degree $2\bar{s}$, and thus

$$\begin{aligned} a_{2s,-1}(z) &= k(z-1)^{\bar{s}}(z+1)^{\bar{s}}, \\ b_{2s,-1}(z) &= 0 \end{aligned} \tag{9}$$

for some $k \neq 0$. If $n \neq -1$, then $a_{mn}^{(1)}(z)$ and $b_{mn}^{(1)}(z)$ satisfy the equality conditions of the lemma with $s = \bar{s} - 1$; thus by the uniqueness result it must be the case that

$$\begin{aligned} a_{mn}^{(1)}(z) &= ka_{m-1,n-1}(z), \\ b_{mn}^{(1)}(z) &= kb_{m-1,n-1}(z), \end{aligned} \tag{10}$$

for some $k \neq 0$. From (10) we get $a_{mn}(z) = a_{mn}(\pm 1) + k\int_{\pm 1}^{z} a_{m-1,n-1}(t)dt$ and $b_{mn}(z) = b_{mn}(\pm 1) + k\int_{\pm 1}^{z} b_{m-1,n-1}(t)dt$. Imposing $a_{mn}(\pm 1) = \pm b_{mn}(\pm 1)$, a simple manipulation of the resulting system gives

$$\begin{aligned} a_{mn}(z) &= kA(z) + \frac{1}{2}k(B(1) - B(-1) - A(1) - A(-1)), \\ b_{mn}(z) &= kB(z) + \frac{1}{2}k(A(1) - A(-1) - B(1) - B(-1)), \end{aligned} \tag{11}$$

with $A(z)$ (resp. $B(z)$) a primitive of $a_{m-1,n-1}(z)$ (resp. $b_{m-1,n-1}(z)$). It is now apparent that the two polynomials are uniquely determined up to the multiplicative constant k. From the inductive hypothesis $a_{m-1,n-1}^{(\bar{s}-1)}(\pm 1) \neq \pm b_{m-1,n-1}^{(\bar{s}-1)}(\pm 1)$, it follows that $a_{mn}^{(\bar{s})}(\pm 1) \neq \pm b_{mn}^{(\bar{s})}(\pm 1)$.

On the other hand, one can easily check that the polynomials defined by the formulas (9) and (11) have degree $\deg(a_{mn}(z)) = m$, $\deg(b_{mn}(z)) = n$ and satisfy (7). So said polynomials exist. □

Proof of Theorem 1. We prove the theorem for a fixed $s > 1$.

We first show that for each $m, n \geqslant 0$ such that $m + n = 2s - 1$ the iteration $z_{k+1} = \varphi_{mn}(z_k)$ is the unique rational iteration of the kind $z_{k+1} = a(z_k)/b(z_k)$ such that $\deg(a(z)) = m$ and $\deg(b(z)) = n$, satisfying **O2** and whose order of local convergence is exactly s (thus it satisfies **O1** as well). Then, we show that any rational iteration satisfying **O1** and **O2** is of the type $z_{k+1} = \varphi_{mn}(z_k)$ for $m+n = 2s-1$.

Let m and n be such that $m + n = 2s - 1$, with $m, n \geqslant 0$; then, by Lemma 3, there are two polynomials $a_{mn}(z)$ and $b_{mn}(z)$ such that $\deg(a_{mn}(z)) = m$, $\deg(b_{mn}(z)) = n$ satisfying (7) and (8). Since $s > 1$, Lemma 2 implies that for $\psi_{mn}(z) := a_{mn}(z)/b_{mn}(z)$ the iteration $z_{k+1} = \psi_{mn}(z_k)$ converges locally to 1 and -1 with order exactly s, thus ψ_{mn} satisfies **O1**.

On the other hand, consider an iteration function $\psi(z) = a(z)/b(z)$ providing a sequence converging with order at least s. By Lemma 2, it follows that conditions (7) hold and thus $\deg(a(z)) + \deg(b(z)) \geqslant 2s-1 = \deg(a_{mn}(z)) + \deg(b_{mn}(z))$ by Lemma 3. Therefore the iteration $z_{k+1} = \psi_{mn}(z_k)$ satisfies **O2**. By the same lemma, equality holds if and only if $a(z)$ and $b(z)$ differ from $a_{mn}(z)$ and $b_{mn}(z)$ by the same multiplicative factor, i.e., when $\psi(z)$ and $\psi_{mn}(z)$ coincide. Thus, this is the unique iteration satisfying both **O1** and **O2** of the kind $z_{k+1} = a(z_k)/b(z_k)$ with $\deg(a(z)) = m$ and $\deg(b(z)) = n$.

Now we show that $\psi_{mn}(z)$ coincides with $\varphi_{mn}(z)$. Since the numerator of $\varphi_{mn}(z)$ has degree m and its denominator has degree n, it is enough to prove that $z_{k+1} = \varphi_{mn}(z_k)$ satisfies **O1** (thus **O2**, in view of Lemma 3).

(a) Odd m, $m = 2m_1 + 1$, $n = 2n_1$. Let $h_{\mu\ell}(\zeta) := P_{\mu\ell}(\zeta)/Q_{\mu\ell}(\zeta)$ be the (μ, ℓ) Padé approximant to $(1-\zeta)^{-1/2}$. Then, in a neighborhood of $\zeta = 0$,

$$h_{\mu\ell}(\zeta) - (1-\zeta)^{-1/2} = O(\zeta^{\mu+\ell+1}).$$

Since $\varphi_{mn}(z) = zh_{m_1,n_1}(1-z^2)$ and $m_1 + n_1 = s - 1$, we get $\varphi_{mn}(z) - z(z^2)^{-1/2} = O((1-z^2)^s)$, for z sufficiently close to 1 or -1. Since $(1-z^2)^s = O((z-1)^s)$ and $(1-z^2)^s = O((z+1)^s)$ in a neighborhood of 1 and -1 respectively, it holds that

$$\begin{aligned} \varphi_{mn}(z) - 1 &= O((z-1)^s), \quad \text{for } z \text{ in a neighborhood of } 1, \\ \varphi_{mn}(z) + 1 &= O((z+1)^s), \quad \text{for } z \text{ in a neighborhood of } -1, \end{aligned} \tag{12}$$

and then $z_{k+1} = \varphi_{mn}(z)$ verifies **O1**.

(b) Even m, $m = 2m_1$, $n = 2n_1 + 1$. By a reasoning similar to case a, we use the (μ, ℓ) Padé approximant to $(1-\zeta)^{1/2}$, say $\tilde{h}_{\mu\ell}(\zeta)$, and $\varphi_{mn}(z) = \tilde{h}_{m_1,n_1}(1-z^2)/z$, thus $\varphi_{mn}(z)$ verifies (12) as well and $z_{k+1} = \varphi_{mn}(z)$ verifies **O1**.

Thus, for each m, n such that $m + n = 2s - 1$, we have $\varphi_{mn}(z) = \psi_{mn}(z)$ and the iteration $z_{k+1} = \varphi_{mn}(z_k)$ is the unique iteration satisfying **O1** and **O2** and whose numerator has degree m and denominator has degree n.

Let $w_{k+1} = a(w_k)/b(w_k)$ be a rational iteration satisfying **O1** and **O2**. Let $m' = \deg(a(z))$ and $n' = \deg(b(z))$. By Lemmas 2 and 3 one has $m' + n' \geqslant 2s - 1$. We claim that $m' + n' = 2s - 1$; if on the contrary $m' + n' > 2s - 1$ then there exist $m \leqslant m'$ and $n \leqslant n'$ such that $m + n = 2s - 1$ and $z_{k+1} = \varphi_{mn}(z_k)$ satisfies **O1**, thus $w_{k+1} = a(w_k)/b(w_k)$ cannot satisfy **O2** and we get a contradiction. Finally, by the aforementioned uniqueness result we conclude that $a(z)/b(z)$ must coincide with $\varphi_{m',n'}(z)$ up to a multiplicative factor. $\square$

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