Robust Padé approximants may have spurious poles

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Abstract

We show that robust Padé approximants obtained with the SVD may have spurious poles and may not converge pointwise.

1 Introduction

In the recent article [3], Gonnet et al. explain how to use the SVD to compute Padé approximants in floating point arithmetic or for problems with noise, and a similar strategy was proposed in [4]. According to [3], “we can reduce the effects of noise, whether intrinsic to the data or introduced by rounding errors,” by decreasing the degree of the approximants when we detect that some singular values of a certain matrix are below a threshold. Experiments suggest that these techniques lead to fewer Froissart doublets and better approximants.

In view of the success of their method in practice, Gonnet et al. asked whether, from the theoretical point of view, their technique leads to rational approximants for which we can prove pointwise convergence. If this were the case then these approximants would have better theoretical properties than Padé’s, because we only have proofs of convergence in capacity for Padé approximants and there are examples in which they diverge for all $z \neq 0$ (see [5].)

In this short note we present an adaptation of the classic example by Gamme [1] which shows that the answer to the open question of Gonnet et al. is negative. In fact, in the next section we show that a sequence of approximants generated by the techniques proposed in [3] may not converge pointwise to the function being approximated, and may have spurious poles even when the matrices involved in their computation have condition number smaller than 5.

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2 Divergence and spurious poles with well-conditioned matrices $B_n$

We consider only Padé approximants of the form $r_n = p_n/q_n$ and write

$$p_n(z) = \sum_{j=0}^{n} a_j z^j$$ and $$q_n(z) = \sum_{j=0}^{n} b_j z^j,$$

with $a := (a_0, \ldots, a_n)^t$ and $b := (b_0, \ldots, b_n)^t$. To compute the approximant for $f = \sum_{k=0}^{\infty} c_k z^k$ we solve the system $B_n b = 0$ and set $a = A_n b$, for

$$A_n := \begin{bmatrix} c_0 & 0 & \cdots & 0 \\ c_1 & c_0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ c_n & c_{n-1} & \cdots & c_0 \end{bmatrix},$$

and

$$B_n := \begin{bmatrix} c_{n+1} & c_n & c_{n-1} & \cdots & \cdots & c_1 \\ c_{n+2} & c_{n+1} & c_n & c_{n-1} & \cdots & c_2 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ c_{2n-1} & c_n & c_{n-1} & c_0 \end{bmatrix}.$$  \hfill (1)

Gonnet et al. \cite{3} are concerned with the case in which $B_n$ is ill-conditioned. In this case, they propose techniques to reduce $n$ and obtain better approximants. Unfortunately, the ill-conditioning of $B_n$ is not the only cause of divergence of Padé approximants, and \cite{3} solves only part of the problem. Of course, this part is important in practice. However, we now present examples showing that more is needed in order to eliminate spurious poles and obtain rational approximants which converge pointwise to $f$.

Our examples are related to the classic one by Gammel \cite{1}, in which $f$ has the form

$$f(z) = 1 + \sum_{k=1}^{\infty} \alpha_k \left( \sum_{n=n_k}^{2n_k} \left( z/z_k \right)^n \right) = 1 + \sum_{k=0}^{\infty} \alpha_k \left( \frac{z/z_k}{1 - z/z_k} \right)^{n_k + 1},$$ \hfill (2)

where $n_k = 2^k - 1$ and the $\alpha_k$ are chosen in order to enforce the convergence of the series above. Gammel's example does not yield a negative answer to the open question by Gonnet et al., because the matrices $B_n$ they lead to may be ill-conditioned. However, if instead of asking for an entire function we content ourselves with $f$ for which the series $f(z) = \sum_{j=0}^{\infty} c_j z^j$ converges for $|z| < 1$, then the function $f$ with the slightly different form

$$f(z) := 1 + \sum_{k=2}^{\infty} 16^k \left( z^{n_k - 1} + z_k^{2n_k} \left( \frac{z/z_k}{1 - z/z_k} \right)^{n_k + 1} \right), \ n_k := 2^k - 2,$$ \hfill (3)
for any sequence \( \{z_k, k \in \mathbb{N}\} \) with \( 0 < |z_k| < 1/3 \), leads to an example in which the matrix \( B_n \) is well-conditioned, the denominator \( q_{n_k}(z) \) is equal to \( 1 - z/z_k \) and \( p_{n_k}(z_k) \neq 0 \). The \((n_k, n_k)\) Padé approximant of the function \( f \) in (3) has a spurious pole at \( z_k \), and the sequence of approximants do not converge uniformly in any set \( A \) such that the interior of \( A_{1/3} := A \cap \{|z| < 1/3\} \) is nonempty and \( \{z_k, k \in \mathbb{N}\} \) is dense in \( A_{1/3} \). Moreover, when each element in the sequence \( \{z_k, k \in \mathbb{N}\} \) is repeated infinitely many times, we do not have pointwise convergence at the \( z_k \), because the \((n_k, n_k)\) Padé approximant assumes the value \( \infty \) at \( z_k \). For example, if the points \( z_k \) are

\[
\frac{1}{4}, \frac{1}{4}, \frac{1}{5}, \frac{1}{5}, \frac{1}{6}, \ldots, \frac{1}{n}, \frac{1}{n}, \frac{1}{n}, \frac{1}{n} + 1, \ldots
\]

then we do not have pointwise convergence at anyone of them.

We now formalise the arguments above, and after that we present our acknowledgements and comments regarding a related article.

**Theorem 1.** If the points \( z_k \in \mathbb{C} \) are such that \( 0 < |z_k| < 1/3 \), then the coefficients \( c_j \) in the expansion \( f(z) = \sum_{j=0}^{\infty} c_j z^j \) of the function \( f \) in (3) are such that \( 0 < |c_j| \leq (j + 3)^4 \) for \( j = 2, 3, 4, \ldots \) and

(i) The function \( f \) has a \((n_k, n_k)\) Padé approximant with \( q_{n_k}(z) = 1 - z/z_k \) and \( p_{n_k}(z_k) \neq 0 \).

(ii) The singular values \( \sigma_1(B_n) \) and \( \sigma_n(B_n) \) of the matrix \( B_n \) in (1) corresponding to \( n = n_k \) satisfy \( \sigma_1(B_n) < 5\sigma_n(B_n) \).

**Proof.** Inspecting (3), the reader will notice that \( c_0 = 1 \) and, for \( k = 2, 3, \ldots \),

\[
c_{2^k-3} = 16^k \quad \text{and} \quad c_j = 16^k z_k^{2^{k+1}-j} \quad \text{for} \quad 2^k - 2 \leq j \leq 2^{k+1} - 4. \tag{4}
\]

Since \( |z_k| < 1 \) it follows that, for \( j \) in (4), we have \( |c_j| \leq 16^k = (2^k)^4 \leq (j + 3)^4 \).

We can rewrite the function \( f \) in (3) as

\[
f(z) = \frac{p_{n_k}(z)}{1 - z/z_k} + O(z^{2n_k+1})
\]

for

\[
p_{n_k}(z) := \left( 1 + \sum_{j=2}^{n_k-1} 16^j \left( z^{n_j-1} + z^{2n_k} \sum_{t=n_j}^{2n_k} \left( \frac{z}{z_j} \right)^t \right) \right) \left( 1 - \frac{z}{z_k} \right)
\]

\[+16^k \left( z^{n_k-1} - \frac{z^{n_k}}{z_k} + (zz_k)^{n_k} \right),
\]

and the accuracy-through-order criterion shows that \( q_{n_k}(z) = 1 - z/z_k \) and \( p_{n_k}(z) \) define the \((n_k, n_k)\) Padé approximant of \( f \). It follows that \( p_{n_k}(z_k) = 16^k z_k^{2n_k} \neq 0 \), and we have proved item (i) in Theorem 1.
In order to verify item (ii), let us show that the matrix $B_n$ corresponding to $n = n_k = 2^k - 2$ has appropriate singular values. Equation (4) shows that $c_{n-1} = c_{2^k-3} = c_{2n} = 16^k$, and we can write

$$B_n = 16^k U + V$$

with

$$V := c_n V_0 + \sum_{j=2}^{n-1} c_{n-j} V_j + \sum_{j=1}^{n-1} c_{n+j} W_j,$$

where $U$, $V_j$ and $W_j$ are $n \times (n + 1)$ matrices such that

- $u_{n1} = u_{i(i+2)} = 1$ for $i = 1, \ldots, n - 1$, and $u_{ij} = 0$ otherwise,
- $(w_j)_{i(i+j+1)} = 1$ for $i = 1, \ldots, n - j$, and $(w_j)_{ik} = 0$ otherwise,
- $(w_j)_{i(i-j+1)} = 1$ for $i = j, \ldots, n$, and $(w_j)_{ik} = 0$ otherwise.

The matrix $U$ has singular values $\sigma_1(U) = \sigma_2(U) = \cdots = \sigma_n(U) = 1$, because $UU^t = I_n$, and $\|V_j\|_2 = \|W_j\|_2 = 1$. It follows that

$$\|V\|_2 \leq S := |c_n| + \sum_{j=1}^{n-2} |c_j| + \sum_{j=n+1}^{2n-1} |c_j| = \sum_{j=1}^{n-2} |c_j| + \sum_{j=n}^{2n-1} |c_j|$$

(5)

and

$$16^k - S \leq \sigma_n(B_n) \leq \sigma_1(B_n) \leq 16^k + S,$$

(6)

due to the inequality $|\sigma_i(M + \Delta) - \sigma_i(M)| \leq \|\Delta\|_2$, which follows from the min/max characterization of the singular values of the $n \times m$ matrix $M$ with $m \geq n$:

$$\sigma_i(M) = \min_{\dim(S) = m-i+1} \left( \max_{\|x\|_2 = 1, x \in S} \|Mx\|_2 \right),$$

where the minimum is taken over all subspaces $S$ of $\mathbb{R}^m$ with dimension $m-i+1$. Recalling that $n = 2^k - 2$ and $|z_k| < 1/3$, we deduce from (7) that

$$\sum_{j=n}^{2n-1} |c_j| = 16^k \sum_{j=2}^{2^k-2} |z_k|^{2^{k+1} - 4 - j} = 16^k \sum_{j=2}^{2^k-2} |z_k|^{2^{k+1} - 4 - j}$$

(7)

$$= 16^k \sum_{m=1}^{\infty} |z_m|^m < 16^k \sum_{m=1}^{\infty} |z_m|^m = \frac{16^k |z_k|}{1 - |z_k|} < \frac{16^k}{2}. $$

Moreover, using (4) we obtain

$$\sum_{j=1}^{n-2} |c_j| = \sum_{m=2}^{k-1} \sum_{j=2^m-3}^{2^m-4} |c_j| = \sum_{m=2}^{k-1} 16^m \left( 1 + \sum_{j=2^m-2}^{2^{m+1}-4} |z_m|^{2^{m+1} - 4 - j} \right)$$

(8)

$$= \sum_{m=2}^{k-1} 16^m \left( 1 + \sum_{l=0}^{2^{m-2}} |z_m|^l \right) < \sum_{m=2}^{k-1} 16^m \left( 1 + \sum_{l=0}^{\infty} |z_m|^l \right)$$

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\[ \sum_{m=2}^{k-1} 16^m \left( 1 + \frac{1}{1 - |z_m|} \right) < \frac{5}{2} \sum_{m=2}^{k-1} 16^m < \frac{5 \cdot 16^k}{2 \cdot 15} = \frac{16^k}{6}. \]

Equations (5), (7) and (8) show that \( S < 2 \cdot 16^k / 3 \). Thus, (6) yields

\[ \frac{\sigma_1(B_n)}{\sigma_n(B_n)} < \frac{1 + \frac{3}{5}}{1 - \frac{3}{5}} = 5 \]

and we are done. \( \square \)

3 Acknowledgments and related work

We would like to thank both referees for reviewing our work. In particular, the first referee called our attention for the similarity between our example and Gammel’s. The first version of this note was based only in [5], and our function \( f \) was described in terms of the coefficients \( c_j \). We were not aware of the explicit formula (2), which lead us to write our examples as in equation (3) in the present version. This formula gives a clearer view of the block structure of the Padé approximants in our example, and this contribution by the first referee was much appreciated.

Finally, we would like to call the reader’s attention to the related article [2], which presents the results of numerical experiments regarding the specific problem we discuss here, and proves theoretical results regarding several problems that we did not address. [2] does not present theoretical examples like ours, but it is broader than this short note.

References

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