An Estimate for the Norm of the Denominator of a Padé Approximation

Hans-Eberhard Scholz

Abstract

For A-acceptable Padé approximations to the exponential function e^z up to the order 18, the norm of the denominator in the half-plane $\mathrm{Re}z \leq \mu \leq 0$ is estimated. If one solves an initial value problem for a semi-linear ordinary differential equation with a numerical method which has such a Padé approximation as stability function, this estimate is needed to examine the contractivity of the numerical solution.

Key words. Padé approximation, implicit Taylor series methods, semi-linear ODEs

AMS(MOS) subject classifications. 65L05, 65L20

When solving the linear initial value problem

$$y' = A\,y, \quad y(x_0) = y_0 \in \mathbb{R}^m \tag{1}$$

with a numerical method with stability function $R(z)$ and stepsize h, then for all $n = 0, 1, \ldots$

$$y_{n+1} = R(hA)\,y_n \tag{2}$$

holds. If the solution of (1) is contractive, i.e. we have $\|y(x_2)\| \leq \|y(x_1)\|$ for all $x_1 \leq x_2$, then it is desirable that the same property for the numerical solution is valid. From (2) we get

$$\|y_{n+1}\| \leq \|R(hA)\|\|y_n\|$$

and contractivity is assured if $\|R(hA)\| \leq 1$.

In general to estimate $\|R(hA)\|$ is not an easy task. Let $\langle \cdot, \cdot \rangle$ denote a scalar product and $\| \cdot \|$ the corresponding vector norm. If the matrix A satisfies

$$\langle Au, u \rangle \leq \mu \|u\|^2 \quad \text{for all} \quad u \in \mathbb{R}^m \tag{3}$$

and if $R(z)$ is a rational function, bounded for Re $z \leq h\mu$, then in the corresponding operator norm we have (cf. e.g. [2] or [4])

$$\|R(hA)\| \leq \sup_{\mathrm{Re} z \leq h\mu} |R(z)|.$$

The (implicit) Taylor series method, other names are Hermite-Taylor, Obreschkoff or HOP method, has

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

with

$$P_{pq}(z) = \sum_{j=0}^{p} \frac{z^j}{j!} \frac{\binom{p}{j}}{\binom{p+q}{j}} \qquad \text{and} \qquad Q_{pq}(z) = \sum_{j=0}^{q} \frac{(-z)^j}{j!} \frac{\binom{q}{j}}{\binom{p+q}{j}} \tag{4}$$

as stability function (cf. e.g. [5], [3] or [1]). $R_{pq}(z)$ is the (p,q)-Padé approximation to the exponential function e^z. This method has the order of consistency $p + q$ and is A-stable for $0 \leq q - p \leq 2$.

If one solves an initial value problem with such a method for the semi-linear equation

$$y' = A\,y + g(x,y),$$

again with stepsize h, then for the examination of the contractivity one needs not only an estimate for $\|R_{pq}(hA)\|$, but also an estimate for $\|Q_{pq}(hA)^{-1}\|$.

Theorem. *For all* $0 \le p, q \le 10$ *with* $0 \le q - p \le 2$ *we have*

$$\min_{Rez \le \nu \le 0} |Q_{pq}(z)| = Q_{pq}(\nu).$$

Proof. If we put

$$\beta_j = \beta_j(p,q) = \frac{1}{j!}\frac{\binom{q}{j}}{\binom{p+q}{j}}$$

as an abbreviation, then for

$$z = x + i\,y = r\,e^{i\,\varphi}$$

we get

$$\begin{aligned}
|Q_{pq}(z)|^2 &= \sum_{j=0}^{q} \sum_{k=0}^{q} (-1)^{j+k} \beta_j\,\beta_k\,r^{j+k}\,e^{i(j-k)\,\varphi}, \\
&= \sum_{j=0}^{q} (-1)^j\,r^j \sum_{k=0}^{2k\le j} 2^{\mathrm{sign}(j-2k)} \beta_k\,\beta_{j-k} \cos((j-2k)\,\varphi) \\
&\qquad + \mathrm{sign}(q) \sum_{j=q+1}^{2q} (-1)^j\,r^j \sum_{k=0}^{2\,k\le 2q-j} 2^{\mathrm{sign}(2q-j-2k)} \\
&\qquad\qquad \cdot \beta_{q-k}\,\beta_{j-q+k} \cos((2q-j-2k)\,\varphi)
\end{aligned}$$

from (4). Because of

$$\cos(k\,\varphi) = \sum_{l=0}^{2l\le k} (-1)^l \binom{k}{2l} \cos^{k-2l}\varphi\ \sin^{2l}\varphi,$$

$$= \sum_{l=0}^{2l\le k} (-1)^l \binom{k}{2l} \cos^{k-2l}\varphi\,(1-\cos^2\varphi)^l,$$

$$= \sum_{l=0}^{2l\le k} (-1)^l \binom{k}{2l} \cos^{k-2l}\varphi \sum_{m=0}^{l} \binom{l}{m}(-1)^m \cos^{2m}\varphi,$$

$$= \sum_{l=0}^{2l\le k} (-1)^l \sum_{m=0}^{2(l+m)\le k} \binom{k}{2l+2m}\binom{l+m}{m} \cos^{k-2l}\varphi$$

it follows further that

$$\begin{aligned} |Q_{pq}(z)|^2 = {} & \sum_{j=0}^{q} (-1)^j\, r^j \sum_{k=0}^{2k\le j} \sum_{l=0}^{k} (-1)^{k+l}\, 2^{\mathrm{sign}(j-2l)} \beta_{j-l}\,\beta_l \\ & \times \sum_{m=0}^{2(k+m)\le j} \binom{j-2l}{2k-2l+2m}\binom{k-l+m}{m} \cos^{j-2k}\varphi \\ & + \ \mathrm{sign}(q) \sum_{j=q+1}^{2q} (-1)^j\, r^j \sum_{k=0}^{2k\le 2q-j} \sum_{l=0}^{k} (-1)^{k+l}\, 2^{\mathrm{sign}(2q-j-2l)} \beta_{q-l}\,\beta_{j-q+l} \\ & \times \sum_{m=0}^{2(k+m)\le 2q-j} \binom{2q-j-2l}{2k-2l+2m}\binom{k-l+m}{m} \cos^{2q-j-2k}\varphi. \end{aligned}$$

With the abbreviations of

$$a_{jkl} = \sum_{m=0}^{2(k+m)\le j} \binom{j-2l}{2k-2l+2m}\binom{k-l+m}{m}$$

$$\text{for} \quad j=0,\ldots,q, \quad 0\le 2k\le j, \quad l=0,\ldots,k,$$

$$b_{jk} = b_{jk}(p,q) = \sum_{l=0}^{k} (-1)^{k+l}\, 2^{\mathrm{sign}(j-2l)} \beta_{j-l}\,\beta_l\, a_{jkl}$$

$$\text{for} \quad j=0,\ldots,q, \quad 0\le 2k\le j,$$

and

$$c_{jk} = c_{jk}(p,q) = \sum_{l=0}^{k} (-1)^{k+l}\, 2^{\mathrm{sign}(j-2l)} \beta_{q-l}\,\beta_{q-j+l}\, a_{jkl}$$

$$\text{for} \quad j = 0, \ldots, q-1, \quad 0 \le 2k \le j,$$

we finally arrive at

$$|Q_{pq}(z)|^2 = \sum_{j=0}^{q} (-1)^j \, r^j \sum_{k=0}^{2k \le j} b_{jk} \cos^{j-2k} \varphi$$
$$+ \operatorname{sign}(q) \sum_{j=0}^{q-1} (-1)^{2q-j} \, r^{2q-j} \sum_{k=0}^{2k \le j} c_{jk} \cos^{j-2k} \varphi$$

and

$$|Q_{pq}(z)|^2 = \sum_{j=0}^{q} (-1)^j \sum_{k=0}^{2k \le j} (x^2+y^2)^k x^{j-2k} b_{jk}$$
$$+ \operatorname{sign}(q) \sum_{j=0}^{q-1} (-1)^{2q-j} \sum_{k=0}^{2k \le j} (x^2+y^2)^{q-j+k} x^{j-2k} c_{jk}.$$

In the appendix, tables of the modified coefficients

$$\tilde{b}_{jk} = \frac{\binom{p+q}{k}}{\binom{p}{k}} \, b_{jk}$$

and

$$\tilde{c}_{jk} = \frac{((p+q)!)^2}{p! \, q!} \, c_{jk}$$

are given. From these tables we see that for the p and q in which we are interested, the c_{jk} and b_{jk} are non-negative. $\square$

For Re $z \le 0$ the function $Q_{pq}(z)^{-1}$ is bounded and rational, so it follows

Corollary. *Assume that the matrix A satisfy (3) and $h\mu \le 0$. Then for all $0 \le p, q \le 10$ with $0 \le q - p \le 2$ we have*

$$\|Q_{pq}(hA)^{-1}\| \le \sup_{Rez \le h\mu} |Q_{pq}(z)^{-1}| = Q_{pq}(h\mu)^{-1}.$$

$\square$

Remark. Looking at it from the numerical point of view, the here given estimates for A-stable implicit Taylor series methods up to order 18 should be sufficient. Usually, stiff differential equations are solved with lower order methods. But for larger p and q the coefficients b_{jk} and c_{jk} are also non-negative. In order not to waste too much space they are given here only for $0 \leq j \leq 10$. Experiments with the symbolic manipulation package Maple suggest that for all $j > 1$ and $0 \leq 2k \leq j$

$$b_{jk} = 2\frac{a_{jk0}}{(j-1-k)!\,j}\frac{\binom{p}{k}}{\binom{p+q}{k}}\frac{q!}{(q-j+k)!}\frac{(p+q-j)!}{(p+q)!}$$

and

$$c_{jk} = 2\frac{a_{jk0}}{(j-1-k)!\,j}\frac{p!\,q!}{((p+q)!)^2}\frac{(p+j-k)!}{(q-j+k)!}\frac{(p+j-q)!}{(p+j-k-q)!}$$

holds, so that the estimates probably apply to A-stable Taylor series methods of any order.

Appendix

Table of the coefficients $\tilde{b}_{jk}$ for $0 \le j \le 10,\ \ 0 \le k \le 2j$

$$\tilde{b}_{00} = 1$$

$$\tilde{b}_{10} = 2\frac{q}{p+q}$$

$$\tilde{b}_{20} = 2\frac{\binom{q}{2}}{\binom{p+q}{2}} \qquad \tilde{b}_{21} = \frac{q}{(p+q-1)(p+q)}$$

$$\tilde{b}_{30} = \frac{4}{3}\frac{\binom{q}{3}}{\binom{p+q}{3}} \qquad \tilde{b}_{31} = 2\frac{q!}{(q-2)!}\frac{(p+q-3)!}{(p+q)!}$$

$$\tilde{b}_{40} = \frac{2}{3}\frac{\binom{q}{4}}{\binom{p+q}{4}} \qquad \tilde{b}_{41} = 2\frac{q!}{(q-3)!}\frac{(p+q-4)!}{(p+q)!} \qquad \tilde{b}_{42} = \frac{1}{2}\frac{q!}{(q-2)!}\frac{(p+q-4)!}{(p+q)!}$$

$$\tilde{b}_{50} = \frac{4}{15}\frac{\binom{q}{5}}{\binom{p+q}{5}} \qquad \tilde{b}_{51} = \frac{4}{3}\frac{q!}{(q-4)!}\frac{(p+q-5)!}{(p+q)!} \qquad \tilde{b}_{52} = \frac{q!}{(q-3)!}\frac{(p+q-5)!}{(p+q)!}$$

$$\tilde{b}_{60} = \frac{4}{45}\frac{\binom{q}{6}}{\binom{p+q}{6}} \qquad \tilde{b}_{61} = \frac{2}{3}\frac{q!}{(q-5)!}\frac{(p+q-6)!}{(p+q)!} \qquad \tilde{b}_{62} = \frac{q!}{(q-4)!}\frac{(p+q-6)!}{(p+q)!} \qquad \tilde{b}_{63} = \frac{1}{6}\frac{q!}{(q-3)!}\frac{(p+q-6)!}{(p+q)!}$$

$$\tilde{b}_{70} = \frac{8}{315}\frac{\binom{q}{7}}{\binom{p+q}{7}} \qquad \tilde{b}_{71} = \frac{4}{15}\frac{q!}{(q-6)!}\frac{(p+q-7)!}{(p+q)!} \qquad \tilde{b}_{72} = \frac{2}{3}\frac{q!}{(q-5)!}\frac{(p+q-7)!}{(p+q)!} \qquad \tilde{b}_{73} = \frac{1}{3}\frac{q!}{(q-4)!}\frac{(p+q-7)!}{(p+q)!}$$

$$\tilde{b}_{80} = \frac{2}{315}\frac{\binom{q}{8}}{\binom{p+q}{8}} \qquad \tilde{b}_{81} = \frac{4}{45}\frac{q!}{(q-7)!}\frac{(p+q-8)!}{(p+q)!} \qquad \tilde{b}_{82} = \frac{1}{3}\frac{q!}{(q-6)!}\frac{(p+q-8)!}{(p+q)!} \qquad \tilde{b}_{83} = \frac{1}{3}\frac{q!}{(q-5)!}\frac{(p+q-8)!}{(p+q)!}$$

$$\tilde{b}_{84} = \frac{1}{24}\frac{q!}{(q-4)!}\frac{(p+q-8)!}{(p+q)!}$$

$$\tilde{b}_{90} = \frac{4}{2835}\frac{\binom{q}{9}}{\binom{p+q}{9}} \qquad \tilde{b}_{91} = \frac{8}{315}\frac{q!}{(q-8)!}\frac{(p+q-9)!}{(p+q)!} \qquad \tilde{b}_{92} = \frac{2}{15}\frac{q!}{(q-7)!}\frac{(p+q-9)!}{(p+q)!} \qquad \tilde{b}_{93} = \frac{2}{9}\frac{q!}{(q-6)!}\frac{(p+q-9)!}{(p+q)!}$$

$$\tilde{b}_{94} = \frac{1}{12}\frac{q!}{(q-5)!}\frac{(p+q-9)!}{(p+q)!}$$

$$\tilde{b}_{10,0} = \frac{4}{14175}\frac{\binom{q}{10}}{\binom{p+q}{10}} \qquad \tilde{b}_{10,1} = \frac{2}{315}\frac{q!}{(q-9)!}\frac{(p+q-10)!}{(p+q)!} \qquad \tilde{b}_{10,2} = \frac{2}{45}\frac{q!}{(q-8)!}\frac{(p+q-10)!}{(p+q)!} \qquad \tilde{b}_{10,3} = \frac{1}{9}\frac{q!}{(q-7)!}\frac{(p+q-10)!}{(p+q)!}$$

$$\tilde{b}_{10,4} = \frac{1}{12}\frac{q!}{(q-6)!}\frac{(p+q-10)!}{(p+q)!} \qquad \tilde{b}_{10,5} = \frac{1}{120}\frac{q!}{(q-5)!}\frac{(p+q-10)!}{(p+q)!}$$

Table of the coefficients $\tilde{c}_{jk}$ for $0 \le j \le 10,\ \ 0 \le k \le 2j$

$$\tilde{c}_{00} = \frac{p!}{q!}$$

$$\tilde{c}_{10} = 2\frac{(p+1)!}{(q-1!}$$

$$\tilde{c}_{20} = 2\frac{(p+2)!}{(q-2!} \qquad \tilde{c}_{21} = \frac{(p+1)!}{(q-1)!}(p+2-q)$$

$$\tilde{c}_{30} = \frac{4}{3}\frac{(p+3)!}{(q-3)!} \qquad \tilde{c}_{31} = 2\frac{(p+2)!}{(q-2)!}(p+3-q)$$

$$\tilde{c}_{40} = \frac{2}{3}\frac{(p+4)!}{(q-4)!} \qquad \tilde{c}_{41} = 2\frac{(p+3)!}{(q-3)!}(p+4-q) \qquad \tilde{c}_{42} = \frac{1}{2}\frac{(p+2)!}{(q-2)!}\frac{(p+4-q)!}{(p+2-q)!}$$

$$\tilde{c}_{50} = \frac{4}{15}\frac{(p+5)!}{(q-5)!} \qquad \tilde{c}_{51} = \frac{4}{3}\frac{(p+4)!}{(q-4)!}(p+5-q) \qquad \tilde{c}_{52} = \frac{(p+3)!}{(q-3)!}\frac{(p+5-q)!}{(p+3-q)!}$$

$$\tilde{c}_{60} = \frac{4}{45}\frac{(p+6)!}{(q-6)!} \qquad \tilde{c}_{61} = \frac{2}{3}\frac{(p+5)!}{(q-5)!}(p+6-q) \qquad \tilde{c}_{62} = \frac{(p+4)!}{(q-4)!}\frac{(p+6-q)!}{(p+4-q)!} \qquad \tilde{c}_{63} = \frac{1}{6}\frac{(p+3)!}{(q-3)!}\frac{(p+6-q)!}{(p+3-q)!}$$

$$\tilde{c}_{70} = \frac{8}{315}\frac{(p+7)!}{(q-7)!} \qquad \tilde{c}_{71} = \frac{4}{15}\frac{(p+6)!}{(q-6)!}(p+7-q) \qquad \tilde{c}_{72} = \frac{2}{3}\frac{(p+5)!}{(q-5)!}\frac{(p+7-q)!}{(p+5-q)!} \qquad \tilde{c}_{73} = \frac{1}{3}\frac{(p+4)!}{(q-4)!}\frac{(p+7-q)!}{(p+4-q)!}$$

$$\tilde{c}_{80} = \frac{2}{315}\frac{(p+8)!}{(q-8)!} \qquad \tilde{c}_{81} = \frac{4}{45}\frac{(p+7)!}{(q-7)!}(p+8-q) \qquad \tilde{c}_{82} = \frac{1}{3}\frac{(p+6)!}{(q-6)!}\frac{(p+8-q)!}{(p+6-q)!} \qquad \tilde{c}_{83} = \frac{1}{3}\frac{(p+5)!}{(q-5)!}\frac{(p+8-q)!}{(p+5-q)!}$$

$$\tilde{c}_{84} = \frac{1}{24}\frac{(p+4)!}{(q-4)!}\frac{(p+8-q)!}{(p+4-q)!}$$

$$\tilde{c}_{90} = \frac{4}{2835}\frac{(p+9)!}{(q-9)!} \qquad \tilde{c}_{91} = \frac{8}{315}\frac{(p+8)!}{(q-8)!}(p+9-q) \qquad \tilde{c}_{92} = \frac{2}{15}\frac{(p+7)!}{(q-7)!}\frac{(p+9-q)!}{(p+7-q)!} \qquad \tilde{c}_{93} = \frac{2}{9}\frac{(p+6)!}{(q-6)!}\frac{(p+9-q)!}{(p+6-q)!}$$

$$\tilde{c}_{94} = \frac{1}{12}\frac{(p+5)!}{(q-5)!}\frac{(p+9-q)!}{(p+5-q)!}$$

$$\tilde{c}_{10,0} = \frac{4}{14175}\frac{(p+10)!}{(q-10)!} \qquad \tilde{c}_{10,1} = \frac{2}{315}\frac{(p+9)!}{(q-9)!}(p+10-q) \qquad \tilde{c}_{10,2} = \frac{2}{45}\frac{(p+8)!}{(q-8)!}\frac{(p+10-q)!}{(p+8-q)!} \qquad \tilde{c}_{10,3} = \frac{1}{9}\frac{(p+7)!}{(q-7)!}\frac{(p+10-q)!}{(p+7-q)!}$$

$$\tilde{c}_{10,4} = \frac{1}{12}\frac{(p+6)!}{(q-6)!}\frac{(p+10-q)!}{(p+6-q)!} \qquad \tilde{c}_{10,5} = \frac{1}{120}\frac{(p+5)!}{(q-5)!}\frac{(p+10-q)!}{(p+5-q)!}$$

Bibliography

[1] G.F. Corliss, A. Griewank, P. Henneberger, G. Kirlinger, F.A. Potras, and H.J. Stetter, *High-Order Stiff ODE Solvers via Automatic Differentiation and Rational Prediction*, Tech. Report IOKOMO 0296, TU Dresden, 1996.

[2] E. Hairer, G. Bader, and Ch. Lubich, *On the stability of semi-implicit methods for ordinary differential equations*, BIT **22** (1982), 211–232.

[3] E. Hairer, S.P. Nørsett, and G. Wanner, *Solving ordinary differential equations I*, Springer-Verlag, 1987.

[4] E. Hairer and G. Wanner, *Solving Ordinary Differential Equations II*, Springer-Verlag, 1991.

[5] P.J. van der Houwen, *Construction of integration formulas for initial value problems*, North Holland, Amsterdam, 1977.