NORTH-HOLLAND

The Padé Method for Computing the Matrix Exponential

M. Arioli

IAN-CNR
via Abbiategrasso 209
27100 Pavia, Italy

B. Codenotti

IMC-CNR
via S. Maria 46
56125 Pisa, Italy

and

C. Fassino

II Universitá degli studi di Roma
Dipartimento di Matematica
via Ricerca Scientifica 5
00133 Roma, Italy

ABSTRACT

We analyze the Padé method for computing the exponential of a real matrix. More precisely, we study the roundoff error introduced by the method in the general case and in three special cases: (1) normal matrices; (2) essentially nonnegative matrices ($a_{ij} \geq 0$, $i \neq j$); (3) matrices A such that $A = D^{-1}BD$, with D diagonal and B essentially nonnegative.

For these special matrices, it turns out that the Padé method is stable. Finally, we compare the Ward upper bound with our results and show that our bounds are generally tighter.

1. INTRODUCTION AND NOTATION

The study of physical, biological, and economic phenomena or problems of control theory often requires the solution of a system of linear, constant coefficient ordinary differential equations

$$\dot{X}(t) = AX(t), \qquad X(0) = I,$$

where A, $X(t)$, $\dot{X}(t)$ are $n \times n$ matrices, and I is the identity matrix.

LINEAR ALGEBRA AND ITS APPLICATIONS 240:111–130 (1996)

0024-3795/96/$15.00
655 Avenue of the Americas, New York, NY 10010
SSDI 0024-3795(94)00190-0

The matrix exponential, the unique solution of this system, is denoted by e^{At} and can be defined by a power series expansion

$$e^{At} = \sum_{i=0}^{\infty} \frac{(At)^i}{i!}.$$

The importance of the above system justifies the interest in the matrix exponential, but the computation of this matrix function can be very difficult.

There exist several methods for computing e^{At}, or more simply, e^A. We can use techniques for solving systems of differential equations [6], since the matrix exponential is the solution of the differential system defined above, or we can approximate e^A using the definition of the matrix exponential by a expansion series [5, 12]. Moreover, it is possible to employ algorithms based on polynomials of matrices [2, 10] or on splittings and decompositions of the matrix A [3, 4].

In 1978, a survey about the main classes of methods was presented in [5]. In that paper the authors concluded that none of the algorithms appeared to be completely satisfactory, from the viewpoint of numerical stability.

In our work, we examine the Padé method for computing the exponential of a real matrix and present some upper bounds for the roundoff error introduced by the algorithm. Moreover, we present several classes of matrices for which the method is stable, such as:

(1) normal matrices;
(2) essentially nonnegative matrices, that is, matrices $A = (a_{ij})$ such that $a_{ij} \geq 0$ for all $i \neq j$;
(3) matrices of the form $A = DBD^{-1}$, where D is diagonal and B is essentially nonnegative.

Some important matrix classes belong to the class of essentially nonnegative matrices: the nonnegative and the essentially positive matrices.

A matrix $A = (a_{ij})$ is:

(1) nonnegative if $a_{ij} \geq 0$ for all i, j;
(2) essentially positive if it is irreducible and essentially nonnegative.

As reported in [11], the exponential of essentially nonnegative matrices is a nonnegative matrix; moreover, a matrix A is essentially positive if and only if the (i, j)th element of e^{At} is positive for all i, j and for all $t > 0$.

The term "essentially positive" was introduced by Birkhoff and Varga [13] in the study of the numerical solution of the time-dependent multigroup diffusion equations of reactor physics; the essentially positive matrices are also called input-output matrices and Leontieff matrices in economic problems. Moreover, the computation of the matrix exponential of nonnegative matrices arises in Markov chain theory, where it is possible to take advantage of the nonnegativity of the matrix to prove a tight upper bound on the approximation error when Taylor series are used [8]. Finally, in [1] the propagation of the roundoff errors in the methods for the computation of the matrix exponential based on the Taylor series is analyzed by techniques similar to the ones used in the following, proving that these methods are also numerically stable for the class of essentially nonnegative matrices.

The work is organized as follows. In Section 2, the Padé algorithm is presented; in Section 3, the truncation error is analyzed. In Section 4, the error analysis of the Padé method is performed and some special cases are studied. Section 5 contains the experimental results, and in Section 6 a comparison with the Ward upper bounds [12] is reported.

Throughout the paper, we use the following assumption and notation:

(1) all matrices are real;
(2) $|A|$ denotes a matrix whose elements are $|a_{ij}|$;
(3) $|A| < |B|$ means that the relation holds componentwise;
(4) $a_{ij}^{(k)}$ denotes the (i, j)th element of the matrix A^k;
(5) $\|\cdot\|_1$ is the matrix 1-norm, i.e.

$$\|A\|_1 = \max_{1 \leq j \leq n} \sum_{i=1}^{n} |a_{ij}|;$$

(6) $\|\cdot\|_2$ is the usual spectral norm;
(7) $\mathbf{u} = 2^{-t}$ denotes the computer relative precision;
(8) $\doteq$ ($\dot{\leq}$) is equality (inequality) ignoring terms of order equal to or greater than $\mathbf{u}^2$;
(9) $\Lambda(A)$ is the spectrum of the matrix A;
(10) $\alpha(A) = \max\{\mathrm{Re}(\lambda) : \lambda \in \Lambda(A)\}$.

2. THE PADÉ ALGORITHM FOR COMPUTING THE MATRIX EXPONENTIAL

If A is an $n \times n$ matrix, the (p, q) Padé approximation to e^A is defined by ([5])

$$R_{pq}(A) = [D_{pq}(A)]^{-1} N_{pq}(A),$$

where

$$N_{pq}(A) = \sum_{j=0}^{p} \frac{(p+q-j)!p!}{(p+q)!j!(p-j)!} A^j$$

and

$$D_{pq}(A) = \sum_{j=0}^{q} \frac{(p+q-j)!q!}{(p+q)!j!(q-j)!} (-A)^j.$$

As suggested in [5], we use the Padé diagonal approximation, that is, $p = q$. In fact, if $p < q$ (or $p > q$), about qn^3 (or pn^3) flops are required for computing $R_{pq}(A)$, and the approximation order is $p + q$, but with the same complexity we can compute $R_{qq}(A)$, whose approximation order is $2q > p + q$.

As reported in [12], the roundoff error introduced when computing R_{qq} (B) increases as the norm of B increases. For this reason, we approximate e^A by $[R_{qq}(A/m)]^m$, where m is the minimum integer such that $\|A/m\|_1 < 0.5$.

From now on, we denote $D_{qq}(A)$, $N_{qq}(A)$, $R_{qq}(A)$ by $D_q(A)$, $N_q(A)$, $R_q(A)$, respectively.

The Padé method for computing the matrix exponential of an arbitrary $n \times n$ matrix A can be organized as follows.

1. If $\|A\|_1 < 0.5$, go to step 4.
2. Determine the minimum integer m such that $\|A\|_1/m < 0.5$.
3. Compute $A := A/m$.
4. Compute $N_q(A)$ and $D_q(A)$.
5. Compute $e^A := [D_q(A)]^{-1}N_q(A)$, by solving the system $D_q(A)e^A = N_q(A)$ using Gaussian elimination with the iterative refinement.
6. If steps 2, 3 were not skipped, compute $e^A := (e^A)^m$. In order to reduce the number of matrix multiplications, choose $m = 2^k$; $e^A := (e^A)^{2^k}$ is obtained by squaring e^A k times.

In order to evaluate the roundoff error of the Padé method, we analyze the error introduced by the steps of the previous algorithm; we assume that only steps 4, 5, 6 introduce errors.

The study of the errors introduced when computing the matrices $N_q(A)$ and $D_q(A)$, solving the system $D_q(A)e^A = N_q(A)$, and squaring the matrix e^A is necessary in order to analyze the total error, but required quite technical proofs. Since the main result—that is, the estimate of the total roundoff error—is reported in Theorem 4.13, the reader who is not interested in the proof can disregard the intermediate results.

3. UPPER BOUND ON THE TRUNCATION ERROR

As reported in [5], the following theorem holds.

THEOREM 3.1. *Let A be an $n \times n$ matrix. If $\|A\|_2/2^j \leq 0.5$, then $[R_{pq}(A/2^j)]^{2^j} = e^{A+E}$, where E is an $n \times n$ matrix and*

$$\|E\|_2 \leq 8\|A\|_2 \left(\frac{\|A\|_2}{2^j}\right)^{p+q} \frac{p!q!}{(p+q)!(p+q+1)!}.$$

This result also holds for the matrix 1-norm. Moreover, from the proof of this theorem (see [5]) we have that the matrices A and E commute and so

$$\frac{\|e^A - e^{A+E}\|_1}{\|e^A\|_1} \leq \|E\|_1 e^{\|E\|_1}.$$

If we choose p and q such that $\|E\|_1$ is less than the computer relative precision, then $e^{\|E\|_1} \simeq 1$ and the relative truncation error is negligible.

4. ROUNDOFF ERROR OF THE PADÉ METHOD

In this section we present some approximate upper bounds on the relative roundoff error for computing the exponential matrix e^A by using the Padé method with diagonal approximants. We assume that operations like scalar by matrix multiplications do not introduce errors.

From now on, we write $\mathrm{fl}(\cdot)$ for the result in floating point computation of that which appears as the argument. More precisely:

(1) the matrices are such that $\mathrm{fl}(A) = A$;
(2) $\mathrm{fl}(A^m)$ is the value obtained by computing A^m using floating point;
(3) $\mathrm{fl}(g(A))$, where $g(A) \in \{R_q(A), N_q(A), D_q(A)\}$, is the value obtained by computing $g(A)$ using floating point;
(4) $\mathrm{fl}(R_q(A/m)^m)$ denotes, for simplicity, the value $\mathrm{fl}(\mathrm{fl}(R_q(A/m))^m)$, i.e., it is the value obtained by computing $\overline{R} = R_q(A/m)$ and $\widetilde{R} = \overline{R}^m$ using floating point.

In order to obtain the upper bounds, we use the absolute value of matrices, $|A| = (|a_{ij}|)$, where

$$|A| < |B|$$

means that the relation holds componentwise.

Let $A, B, A_k, k = 0, \ldots, p$, be $n \times n$ matrices. It is easy to show that

$$|\mathrm{fl}(A+B) - (A+B)| < \mathbf{u}|A+B|, \tag{1}$$

$$|\mathrm{fl}(AB) - (AB)| < \mathbf{u}n|A||B|, \tag{2}$$

$$\left|\mathrm{fl}\left(\sum_{k=0}^{p} A_k\right) - \left(\sum_{k=0}^{p} A_k\right)\right| < \mathbf{u}p\sum_{k=0}^{p}|A_k|, \tag{3}$$

$$|\mathrm{fl}(A^k) - A^k| \dot{\leq} \mathbf{u}n(k-1)|A|^k. \tag{4}$$

REMARK. From (4), we obtain

$$\|\mathrm{fl}(A^k) - A^k\|_1 \dot{\leq} \mathbf{u}n(k-1)\|A\|_1^k.$$

If $\|A\|_1 < 1$, since $\|A\|_1^k < 1$, this can be a good approximate upper bound. But if $\|A\|_1 \geq 1$ and, roughly speaking, A "differs" from the matrix $|A|$, this approximate upper bound can be very large. In that case we can use some other approximate upper bound, presented in one of the following theorems.

THEOREM 4.1. *Let A be an $n \times n$ matrix and let $m = 2^p$. We have*

$$F_p := \mathrm{fl}(A^{2^p}) - A^{2^p} \doteq \sum_{h=1}^{p} \sum_{k=0}^{2^{p-h}-1} A^{2^p - 2^h(k+1)} E_h A^{k2^h},$$

where

$$E_h = \mathrm{fl}(A^{2^h}) - \mathrm{fl}(A^{2^{h-1}})^2 \quad \text{and} \quad |E_h| \dot{\leq} n\mathbf{u}|A^{2^{h-1}}|^2,$$

that is, E_h is a local error of the hth step.

Proof. This result is shown by induction.
$p = 1$: Obvious, because we have

$$\sum_{h=1}^{1} \sum_{k=0}^{2^{1-h}-1} A^{2^p - 2^h(k+1)} E_h A^{k2^h} = E_1 = \mathrm{fl}(A^2) - A^2 = F_1.$$

$p = 2$:

$$\begin{aligned}\sum_{h=1}^{2} \sum_{k=0}^{2^{2-h}-1} A^{4-2^h(k+1)} E_h A^{k2^h} &= A^2E_1 + E_1A^2 + E_2 \\ &\doteq (A^2 + E_1)^2 - A^4 + E_2 \\ &= \mathrm{fl}(A^2)^2 - A^4 + \mathrm{fl}(A^4) - \mathrm{fl}(A^2)^2 = F_2.\end{aligned}$$

We suppose that the result is true for p, and we show that it is true for $p+1$:

$$\begin{aligned}\sum_{h=1}^{p+1}\sum_{k=0}^{2^{p+1-h}-1} & A^{2^{p+1}-2^h(k+1)}E_hA^{k2^h}\\ &= E_{p+1}+\sum_{h=1}^{p}\left[\sum_{k=0}^{2^{p-h}-1}A^{2^{p+1}-2^h(k+1)}E_hA^{k2^h}\right.\\ &\qquad\left.+\sum_{j=2^{p-h}}^{2^{p+1-h}-1}A^{2^{p+1}-2^h(j+1)}E_hA^{j2^h}\right].\end{aligned}$$

After the change $k = j - 2^{p-h}$, we obtain

$$\begin{aligned}E_{p+1}&+\sum_{h=1}^{p}\left[\sum_{k=0}^{2^{p-h}-1}A^{2^{p+1}-2^h(k+1)}E_hA^{k2^h}\right.\\ &\qquad\left.+\sum_{k=0}^{2^{p-h}-1}A^{2^p-2^h(k+1)}E_hA^{2^p+k2^h}\right]\\ &= E_{p+1}+A^{2^p}F_p+F_pA^{2^p}\doteq\left(F_p+A^{2^p}\right)^2+E_{p+1}-\left(A^{2^p}\right)^2\\ &= \mathrm{fl}\left(A^{2^p}\right)^2+E_{p+1}-\left(A^{2^p}\right)^2=\mathrm{fl}\left(A^{2^{p+1}}\right)-A^{2^{p+1}}=F_{p+1}.\end{aligned}$$ ∎

COROLLARY 4.2. *From Theorem* 4.1, *we obtain an approximate upper bound, using the matrix absolute value,*

$$|F_p| = \left|\mathrm{fl}\left(A^{2^p}\right)-A^{2^p}\right| \mathrel{\dot{\le}} n\mathbf{u}\sum_{h=1}^{p}\sum_{k=0}^{2^{p-h}-1}\left|A^{2^p-2^h(k+1)}\right|\left|A^{2^{h-1}}\right|^2\left|A^{k2^h}\right|.$$

COROLLARY 4.3. *Let A be an $n\times n$ normal matrix, and let $m = 2^p$. We have*

$$\frac{\|\mathrm{fl}(A^m)-A^m\|_1}{\|A^m\|_1}\mathrel{\dot{\le}} n^3\sqrt{n}\mathbf{u}(m-1).$$

Proof. If we use the notation of Theorem 4.1, then since if A is normal $\|A\|_2^k = \|A^k\|_2$, we have

$$\begin{aligned}\|E_h\|_2 &< \sqrt{n}\|E_h\|_1 \mathrel{\dot{\le}} n\sqrt{n}\mathbf{u}\left\|A^{2^{h-1}}\right\|_1^2\\ &< n^2\sqrt{n}\mathbf{u}\left\|A^{2^{h-1}}\right\|_2^2 = n^2\sqrt{n}\mathbf{u}\left\|A^{2^h}\right\|_2,\end{aligned}$$

and so

$$\begin{aligned}\|\mathrm{fl}(A^m) - A^m\|_1 &\dot{\leq} n\mathbf{u}\sum_{h=1}^{p}\sum_{k=0}^{2^{p-h}-1} \|A^{2^p-2^h(k+1)}\|_1 \|A^{2^{h-1}}\|^2\|_1 A^{k2^h}\|_1 \\ &< n^3\mathbf{u}\sum_{h=1}^{p}\sum_{k=0}^{2^{p-h}-1} \|A^{2^p}\|_2 = n^3\mathbf{u}(2^p-1)\|A^{2^p}\|_2 \\ &< n^3\sqrt{n}\mathbf{u}(2^p-1)\|A^{2^p}\|_1,\end{aligned}$$

and we have the result. ■

COROLLARY 4.4. *If A is a nonnegative matrix, we obtain*

$$|F_p| = |\mathrm{fl}(A^m) - A^m| \dot{\leq} n\mathbf{u}(m-1)A^m.$$

COROLLARY 4.5. *Let A be a nonnegative $n \times n$ matrix, and let D be a diagonal nonsingular $n \times n$ matrix. If $B = DAD^{-1}$ and $m = 2^p$, we have*

$$|F_p| = |\mathrm{fl}(B^m) - B^m| \dot{\leq} n\mathbf{u}(m-1)|B^m|.$$

Proof.

$$\begin{aligned}|F_p| &\dot{\leq} n\mathbf{u}\sum_{h=1}^{p}\sum_{k=0}^{2^{p-h}-1} |DA^{2^p-2^h(k+1)}D^{-1}||DA^{2^{h-1}}D^{-1}|^2|DA^{k2^h}D^{-1}| \\ &= n\mathbf{u}\sum_{h=1}^{p}\sum_{k=0}^{2^{p-h}-1} |D|A^{2^p}|D^{-1}| = n\mathbf{u}\sum_{h=1}^{p}\sum_{k=0}^{2^{p-h}-1} |DA^{2^p}D^{-1}| \\ &= n\mathbf{u}(2^p-1)|B^{2^p}|.\end{aligned}$$

■

4.1. Roundoff Error for Computing $D_q(A)$ and $N_q(A)$

We have the following result.

THEOREM 4.6. *Let A be an $n \times n$ matrix. Then*

$$|\mathrm{fl}(D_q(A)) - D_q(A)| \dot{\leq} \mathbf{u}q(n+1)e^{|A|/2},$$

$$|\mathrm{fl}(N_q(A)) - N_q(A)| \dot{\leq} \mathbf{u}q(n+1)e^{|A|/2}.$$

Proof. The proof is carried out for the matrix $D_q(A)$, but the generalization for $N_q(A)$ is easy.

Using the notation $a_j = (2q-j)!q!/(2q)!j!(q-j)!$, we obtain

$$\begin{aligned}
|\mathrm{fl}(D_q) - D_q| &< \left|\mathrm{fl}\left(\sum_{j=0}^{q}(-1)^j a_j A^j\right) - \sum_{j=0}^{q}(-1)^j a_j \mathrm{fl}(A^j)\right| \\
&\quad + \left|\sum_{j=0}^{q}(-1)^j a_j \mathrm{fl}(A^j) - \sum_{j=0}^{q}(-1)^j a_j A^j\right| \\
&< \mathbf{u}\left[q\sum_{j=0}^{q} a_j|\mathrm{fl}(A^j)| + n\sum_{j=0}^{q}(j-1)a_j|A|^j\right] \\
&\dot{\leq} \mathbf{u}q\left[\sum_{j=0}^{q} a_j|A|^j + n\sum_{j=0}^{q} a_j|A|^j\right] \\
&= \mathbf{u}q(n+1)\sum_{j=0}^{q} a_j|A|^j.
\end{aligned}$$

Since $\sum_{j=0}^{\infty} a_j B^j = e^{B/2}$, we can approximate $\sum_{j=0}^{q} a_j|A|^j$ with $e^{|A|/2}$ and so

$$|\mathrm{fl}(D_q) - D_q| \dot{\leq} \mathbf{u}q(n+1)e^{|A|/2}. \qquad \blacksquare$$

4.2. Roundoff Error for Computing $R_q(A)$

By definition the matrix $R_q(A)$ is the solution of the system

$$D_q(A)R_q(A) = N_q(A),$$

but the effect of the roundoff errors is that the computed solution $\mathrm{fl}(R_q(A))$ satisfies

$$[\mathrm{fl}(D_q(A)) + H_j]\mathrm{fl}(R_q(A)^{(j)}) = \mathrm{fl}(N_q(A)^{(j)}) + E^{(j)},$$

where the matrices H_j and E depend on the method chosen for solving the system and $B^{(j)}$ denotes the jth column of the matrix B.

In order to obtain the following results, we use the Skeel theory. If we solve the system $Ax = b$ using iterative refinement, we obtain a vector $\widetilde{x}$, which is the exact solution of $(A+E)\widetilde{x} = b + f$, where $|E| < \omega|A|$, $|f| < \omega|b|$, and $\omega \leq (n+1)\mathbf{u}$ [7]. In practice, we find that the constant ω is less than the machine precision, that is, $\omega < \mathbf{u}$.

THEOREM 4.7. *If E_N and E_D are the roundoff errors for computing the matrices $N_q(A)$ and $D_q(A)$, respectively, if we solve the system*

$D_q(A)R_q(A) = N_q(A)$ *by Gaussian elimination with iterative refinement, then*

$$|\mathrm{fl}(R_q(A)) - R_q(A)| \dot{\leq} \mathbf{u}e^{|A|}[q(n+1)+1][I + |R_q(A)|].$$

Proof.

$$\begin{aligned}\mathrm{fl}(R_q(A))^{(j)} &= [\mathrm{fl}(D_q(A)) + H_j]^{-1}[\mathrm{fl}(N_q(A))^{(j)} + E^{(j)}] \\ &= [D_q(A) + E_D + H_j]^{-1}\big[N_q(A)^{(j)} + E_N^{(j)} + E^{(j)}\big] \\ &= [I + D_q(A)^{-1}E_D + D_q(A)^{-1}H_j]^{-1}D_q(A)^{-1} \\ &\quad \times \big[N_q(A)^{(j)} + E_N^{(j)} + E^{(j)}\big].\end{aligned}$$

We obtain

$$\begin{aligned}&[I + D_q(A)^{-1}E_D + D_q(A)^{-1}H_j]\mathrm{fl}(R_q(A))^{(j)} \\ &\quad = D_q(A)^{-1}\big[N_q(A)^{(j)} + E_N^{(j)} + E^{(j)}\big]\end{aligned}$$

and so

$$\begin{aligned}&\mathrm{fl}(R_q(A))^{(j)} - R_q(A)^{(j)} \doteq D_q(A)^{-1} \\ &\quad \times \big[E_N^{(j)} + E^{(j)} - (E_D + H_j)R_q(A)^{(j)}\big].\end{aligned}$$

The relation between the absolute values is

$$\begin{aligned}&|\mathrm{fl}(R_q(A))^{(j)} - R_q(A)^{(j)}| \dot{\leq} |D_q(A)^{-1}| \\ &\quad \times \big[|E_N^{(j)}| + |E^{(j)}| + (|E_D| + |H_j|)|R_q(A)^{(j)}|\big],\end{aligned}$$

where

$$|H_j| < \mathbf{u}|D_q(A)| \quad \text{and} \quad |E| < \mathbf{u}|R_q(A)|,$$

because we solve the system using iterative refinement, and thus

$$\begin{aligned}&|\mathrm{fl}(R_q(A))^{(j)} - R_q(A)^{(j)}| \\ &\quad \dot{\leq} |D_q(A)^{-1}|\big\{|E_N^{(j)}| + \mathbf{u}|N_q(A)^{(j)}| + [|E_D| + \mathbf{u}|D_q(A)|]|R_q(A)^{(j)}|\big\}.\end{aligned}$$

The right-hand side of the previous relation is the jth column of the matrix

$$|D_q(A)^{-1}|\{|E_N| + \mathbf{u}|N_q(A)| + [|E_D| + \mathbf{u}|D_q(A)|]|R_q(A)|\},$$

and so, since, $N_q(A) \approx e^{A/2}$, $D_q(A) \approx e^{-A/2}$, and $D_q(A)^{-1} \approx e^{A/2}$,

$$|\mathrm{fl}(R_q(A)) - R_q(A)| \dot{\leq} |e^{A/2}|[|E_N| + \mathbf{u}|e^{A/2}| + (|E_D| + \mathbf{u}|e^{A/2}|)|R_q(A)|].$$

From Theorem 4.6 our proof follows. ∎

COROLLARY 4.8. *Let A be an $n \times n$ matrix with 1-norm less than* 0.5. *We have*

$$\frac{\|\mathrm{fl}(R_q(A)) - R_q(A)\|_1}{\|R_q(A)\|_1} \dot{\leq} \mathbf{u}e^{1/2}[q(n+1)+1](1+e^{1/2})$$

Proof. If we replace the absolute value with the matrix norm, from Theorem 4.7 we obtain

$$\|\mathrm{fl}(R_q(A)) - R_q(A)\|_1 \dot{\leq} \mathbf{u}e^{1/2}[q(n+1)+1][1+\|R_q(A)\|_1].$$

As reported in [5], $\|e^A\| > e^{\alpha(A)}$, where $\alpha(A) = \max\{\mathrm{Re}\lambda \mid \lambda \in \Lambda(A)\}$. Since $\|A\|_1 < 0.5\ \forall\lambda \in \Lambda(A)$, we have $|\lambda| < 0.5$ and so $-0.5 < \alpha(A) < 0.5$. We can conclude that

$$\frac{1}{\|R_q(A)\|_1} \approx \frac{1}{\|e^A\|_1} < e^{-\alpha(A)} < e^{1/2},$$

and

$$\begin{aligned}\frac{\|\mathrm{fl}(R_q(A)) - R_q(A)\|_1}{\|R_q(A)\|_1} &\dot{\leq} \mathbf{u}e^{1/2}[q(n+1)+1]\left(1+\frac{1}{\|R_q(A)\|_1}\right)\\ &< \mathbf{u}e^{1/2}[q(n+1)+1](1+e^{1/2}).\end{aligned}$$ ∎

4.3. Roundoff Error for Approximating e^A

As reported in [12], the Padé algorithm is stable if the 1-norm of the matrix A is less than 1, and so, if the matrix norm is greater than 1, we must scale it. In this case, we compute the matrix exponential as follows:

$$e^A = (e^{A/m})^m,$$

where m is the minimum integer such that $\|A\|_1/m < 0.5$.

In order to obtain an approximate upper bound for the roundoff error for computing the matrix exponential, we study the error introduced when we compute the powers of a perturbed matrix.

THEOREM 4.9. *Let E_B be the perturbation of a matrix B, and let $\widetilde{B}$ be the perturbed matrix, that is, $\widetilde{B} = B + E_B$. Then we have*

$$\begin{aligned}|\mathrm{fl}(\widetilde{B}^m) - B^m| \;&\dot{\leq}\; \sum_{i=0}^{m-1} |B^i||E_B||B^{m-i-1}|\\ &\quad + n\mathbf{u}\sum_{h=1}^{p}\sum_{k=0}^{2^{p-h}-1} |B^{2^p-2^h(k+1)}||B^{2^{h-1}}|^2|B^{k2^h}|.\end{aligned}$$

Proof.

$$
\begin{aligned}
|\mathrm{fl}(\widetilde{B}^m) - B^m| &= |\mathrm{fl}(\widetilde{B}^m) - \widetilde{B}^m + \widetilde{B}^m - B^m| \\
&< |\mathrm{fl}(\widetilde{B}^m) - \widetilde{B}^m| + |\widetilde{B}^m - B^m| \\
&\doteq |\mathrm{fl}(\widetilde{B}^m) - \widetilde{B}^m| + |(B + E_B)^m - B^m| \\
&\dot{\leq} n\mathbf{u} \sum_{h=1}^{p} \sum_{k=0}^{2^{p-h}-1} |B^{2^p - 2^h(k+1)}||B^{2^{h-1}}|^2 |B^{k2^h}| \\
&\quad + \sum_{i=0}^{m-1} |B^i||E_B||B^{m-i-1}|. \qquad \blacksquare
\end{aligned}
$$

THEOREM 4.10. *Let A be an $n \times n$ matrix, let p be the minimum integer such that $\|A\|_1 < 2^{p-1}$, and let $m = 2^p$. An approximate upper bound for the roundoff error introduced by the Padé method for computing e^A is given as follows, if we use Gaussian elimination with iterative refinement for solving the system:*

$$
\begin{aligned}
&\left|\mathrm{fl}\left(R_q\left(\frac{A}{m}\right)^m\right) - R_q\left(\frac{A}{m}\right)^m\right| \\
&\dot{\leq} n\mathbf{u} \sum_{h=1}^{p} \sum_{k=0}^{2^{p-h}-1} \left|R_q\left(\frac{A}{m}\right)^{2^p - 2^h(k+1)}\right| \left|R_q\left(\frac{A}{m}\right)^{2^{h-1}}\right|^2 \left|R_q\left(\frac{A}{m}\right)^{k2^h}\right| \\
&\quad + \mathbf{u}[q(n+1)+1] \sum_{i=0}^{m-1} \left|R_q\left(\frac{A}{m}\right)^i\right| e^{|A|/m} \\
&\quad \times \left[I + \left|R_q\left(\frac{A}{m}\right)\right|\right] \left|R_q\left(\frac{A}{m}\right)^{m-i-1}\right|.
\end{aligned}
$$

Proof. We obtain this result from Theorems 4.7 and 4.9, since we compute the mth power of the matrix $\mathrm{fl}(R_q(A/m))$ perturbed by the error matrix E_R, and

$$
|E_R| \,\dot{\leq}\, \mathbf{u} e^{|A|/m} [q(n+1)+1] \left[I + \left|R_q\left(\frac{A}{m}\right)\right|\right]. \qquad \blacksquare
$$

Since the exponential of essentially nonnegative matrices is a nonnegative matrix [11], in this case we can compute the matrix power $(e^{A/m})^m$ without cancellations, and so the Padé method is stable. In the following, we examine, in detail, the roundoff error introduced when computing the exponential of essentially nonnegative matrices.

If A is an essentially nonnegative matrix, since $R_q(A/m)$ approximates $e^{A/m}$ with a truncation error less than the machine precision, we can suppose that $R_q(A/m)$ is a nonnegative matrix.

COROLLARY 4.11. *Let A be an $n \times n$ essentially nonnegative matrix. If the same hypotheses of Theorem* 4.10 *holds, we have*

$$\left|\mathrm{fl}\left(R_q\left(\frac{A}{m}\right)^m\right) - R_q\left(\frac{A}{m}\right)^m\right|$$
$$\dot{\leq} \mathbf{u}m\left\{nI + [1 + q(n+1)]e^{|A|/m}\left[I + R_q\left(\frac{A}{m}\right)^{-1}\right]\right\}R_q\left(\frac{A}{m}\right)^m.$$

COROLLARY 4.12. *Let A be an $n \times n$ matrix such that $A = DBD^{-1}$, where B is an essentially nonnegative matrix and D is diagonal. With the same hypotheses of Theorem* 4.10, *we have*

$$\left|\mathrm{fl}\left(R_q\left(\frac{A}{m}\right)^m\right) - R_q\left(\frac{A}{m}\right)^m\right|$$
$$\dot{\leq} \mathbf{u}m\left\{nI + [1 + q(n+1)]e^{|A|/m}\left[I + \left|R_q\left(\frac{A}{m}\right)^{-1}\right|\right]\right\}\left|R_q\left(\frac{A}{m}\right)^m\right|.$$

Proof. From Theorem 4.10 and Corollary 4.5 we have

$$\left|\mathrm{fl}\left(R_q\left(\frac{A}{m}\right)^m\right) - R_q\left(\frac{A}{m}\right)^m\right| < \mathbf{u}n(m-1)\left|R_q\left(\frac{A}{m}\right)^m\right|$$
$$+ \mathbf{u}[q(n+1)+1]\sum_{i=0}^{m-1}\left|R_q\left(\frac{A}{m}\right)^i\right|e^{|A|/m}\left[I + \left|R_q\left(\frac{A}{m}\right)\right|\right]\left|R_q\left(\frac{A}{m}\right)^{m-i-1}\right|.$$

But if $A = DBD^{-1}$, then there exists a nonnegative matrix C such that $R_q(A/m) = DCD^{-1}$, and so

$$\sum_{i=0}^{m-1}\left|R_q\left(\frac{A}{m}\right)^i\right|e^{|A|/m}\left[I + \left|R_q\left(\frac{A}{m}\right)\right|\right]\left|R_q\left(\frac{A}{m}\right)^{m-i-1}\right|$$
$$= |D|\sum_{i=0}^{m-1} C^i e^{B/m}(I+C)C^{m-i-1}|D^{-1}|$$
$$= |D|e^{B/m}C^{m-1}(I+C)|D^{-1}| = e^{|A|/m}\left[\left|R_q\left(\frac{A}{m}\right)^{-1}\right| + I\right]\left|R_q\left(\frac{A}{m}\right)^m\right|.$$

We obtain that

$$\left|\mathrm{fl}\left(R_q\left(\frac{A}{m}\right)^m\right) - R_q\left(\frac{A}{m}\right)^m\right| \dot{\leq} \mathbf{u}n(m-1)\left|R_q\left(\frac{A}{m}\right)^m\right|$$
$$+\mathbf{u}m[1+q(n+1)]e^{|A|/m}\left[\left|R_q\left(\frac{A}{m}\right)^{-1}\right|+I\right]\left|R_q\left(\frac{A}{m}\right)^m\right|,$$

and we have the result. ■

THEOREM 4.13. *Let A be an $n\times n$ matrix, let p be the minimum integer such that $\|A\|_1 < 2^{p-1}$, and let $m = 2^p$. An approximate upper bound for the roundoff error introduced by the Padé method for computing e^A is given as follows, if we use Gaussian elimination with iterative refinement for solving the system.*

(1) *General case*:

$$\left\|\mathrm{fl}\left(R_q\left(\frac{A}{m}\right)^m\right) - R_q\left(\frac{A}{m}\right)^m\right\|_1$$
$$\dot{\leq} n\mathbf{u}\sum_{h=1}^{p}\sum_{k=0}^{2^{p-h}-1}\left\|R_q\left(\frac{A}{m}\right)^{2^p-2^h(k+1)}\right\|_1$$
$$\times\left\|R_q\left(\frac{A}{m}\right)^{2^{h-1}}\right\|_1^2\left\|R_q\left(\frac{A}{m}\right)^{k2^h}\right\|_1$$
$$+\mathbf{u}e^{1/2}[1+q(n+1)](1+e^{1/2})\sum_{i=0}^{m-1}\left\|R_q\left(\frac{A}{m}\right)^i\right\|_1\left\|R_q\left(\frac{A}{m}\right)^{m-i-1}\right\|_1$$

(2) *A is a normal matrix*:

$$\frac{\|\mathrm{fl}(R_q(A/m)^m) - R_q(A/m)^m\|_1}{\|R_q(A/m)^m\|_1}$$
$$\dot{\leq}\mathbf{u}mn^2e^{1/2}[1+q(n+1)](1+e^{1/2})+\mathbf{u}n^3\sqrt{n}(m-1).$$

(3) *A is a essentially nonnegative matrix or $A = DBD^{-1}$, where B is an essentially nonnegative matrix and D is a diagonal matrix:*

$$\frac{\|\mathrm{fl}\,(R_q(A/m)^m) - R_q(A/m)^m\|_1}{\|R_q(A/m)^m\|_1}\dot{\leq}\mathbf{u}m\{n+e^{1/2}[1+q(n+1)](1+e^{3/2})\}.$$

Proof. (1) General case: It is sufficient to replace the absolute value with the matrix norm and to use the approximate upper bound

$$\left\|R_q\left(\frac{A}{m}\right)\right\|_1 \approx \|e^{A/m}\|_1 < e^{\|A/m\|} < e^{1/2}.$$

(2) Normal matrix: We have, from Theorem 4.9, if E_R is the roundoff error introduced when computing $R_q(A/m)$,

$$\begin{aligned}
&\left\| \mathrm{fl}\left(R_q\left(\frac{A}{m}\right)^m\right) - R_q\left(\frac{A}{m}\right)^m \right\|_1 \\
&\quad \dot{\leq} \sum_{i=0}^{m-1} \left\| R_q\left(\frac{A}{m}\right)^i \right\|_1 \|E_R\|_1 \left\| R_q\left(\frac{A}{m}\right)^{m-i-1} \right\|_1 \\
&\quad + n\mathbf{u} \sum_{h=1}^{p} \sum_{k=0}^{2^{p-h}-1} \left\| R_q\left(\frac{A}{m}\right)^{2^p-2^h(k+1)} \right\|_1 \\
&\quad \times \left\| R_q\left(\frac{A}{m}\right)^{2^{h-1}} \right\|_1^2 \left\| R_q\left(\frac{A}{m}\right)^{k2^h} \right\|_1 .
\end{aligned}$$

Since $R_q(A/m)$ is normal, from Corollaries 4.3 and 4.8 we have

$$\begin{aligned}
&\left\| \mathrm{fl}\left(R_q\left(\frac{A}{m}\right)^m\right) - R_q\left(\frac{A}{m}\right)^m \right\|_1 \\
&\quad \dot{\leq} \sum_{i=0}^{m-1} \left\| R_q\left(\frac{A}{m}\right)^i \right\|_1 \|E_R\|_1 \left\| R_q\left(\frac{A}{m}\right)^{m-i-1} \right\|_1 \\
&\quad + \mathbf{u}n^3\sqrt{n}(m-1) \left\| R_q\left(\frac{A}{m}\right)^m \right\|_1 \\
&\quad = \mathbf{u}e^{1/2}[1+q(n+1)](1+e^{1/2}) \sum_{i=0}^{m-1} \left\| R_q\left(\frac{A}{m}\right)^i \right\|_1 \\
&\quad \times \left\| R_q\left(\frac{A}{m}\right) \right\|_1 \left\| R_q\left(\frac{A}{m}\right)^{m-i-1} \right\|_1 \\
&\quad + \mathbf{u}n^3\sqrt{n}(m-1) \left\| R_q\left(\frac{A}{m}\right)^m \right\|_1 \\
&\quad < \mathbf{u}n\sqrt{n}m \left\| R_q\left(\frac{A}{m}\right)^m \right\|_2 e^{1/2}(1+q(n+1))(e^{1/2}+1) \\
&\quad + \mathbf{u}n^3\sqrt{n}(m-1) \left\| R_q\left(\frac{A}{m}\right)^m \right\|_1 \\
&\quad = \mathbf{u}n^2 m \left\| R_q\left(\frac{A}{m}\right)^m \right\|_1 e^{1/2}(1+q(n+1))(e^{1/2}+1) \\
&\quad + \mathbf{u}n^3\sqrt{n}(m-1) \left\| R_q\left(\frac{A}{m}\right)^m \right\|_1 .
\end{aligned}$$

(3) Essentially nonnegative matrix: If A is essentially nonnegative or if $A = DBD^{-1}$, B essentially nonnegative and D diagonal, then from Corollary 4.11 or from Corollary 4.12, respectively, we have

$$\frac{\|\mathrm{fl}\,(R_q(A/m)^m) - R_q(A/m)^m\|_1}{\|R_q(A/m)^m\|_1} \dot{\leq} \mathbf{u}m\left\{n + e^{1/2}[1 + q(n+1)]\left[1 + \left\|R_q\left(\frac{A}{m}\right)^{-1}\right\|_1\right]\right\}.$$

We can conclude, because $\|R_q(A/m)^{-1}\|_1 < e^{3/2}$. In fact

$$\left\|R_q\left(\frac{A}{m}\right)^{-1}\right\|_1 \left\|R_q\left(\frac{A}{m}\right)\right\|_1 \approx \|e^{-A/m}\|_1\|e^{A/m}\|_1 < e^{2\|A\|_1/m} < e,$$

and so

$$\left\|R_q\left(\frac{A}{m}\right)^{-1}\right\|_1 < \frac{e}{\|R_q(A/m)\|_1} < ee^{1/2} = e^{3/2}. \qquad \blacksquare$$

5. COMPARISON WITH THE WARD UPPER BOUNDS

We compare the results presented in the previous theorems with the upper bounds obtained by Ward [12] for the roundoff error of the Padé method. In the upper bounds, Ward also considers the roundoff error introduced by the scalar by matrix products, which we neglect. Moreover, he uses Gaussian elimination for solving the system $D_q(A)R_q(A) = R_q(A)$, whereas we use iterative refinement. These differences experimentally do not appreciably influence the upper bounds mentioned above.

We distinguish several cases.

(1) *The exponential of matrices without special properties.* As reported in [12], Ward obtains the following upper bounds for the roundoff error for computing $R_q(A/m)^m$:

$$\|G_0\|_1 < \mathbf{u}(83.7n + 71.8)\left\|R_q\left(\frac{A}{m}\right)\right\|_1,$$

$$\|G_k\|_1 \dot{\leq} 2\left\|R_q\left(\frac{A}{m}\right)^{2^{k-1}}\right\|_1 \|G_{k-1}\|_1 + \|G_{k-1}\|_1^2 + n\mathbf{u}\left\|R_q\left(\frac{A}{m}\right)^{2^{k-1}}\right\|_1^2,$$

where G_0 is the error introduced when computing $R_q(A/m)$. The Ward upper bound for the total roundoff error of the Padé method is comparable with the approximate upper bound presented in Theorem 4.13(1), but, in general, it is worse.

(2) *The exponential of nonnegative matrices.* The Ward upper bound for the error introduced by the Padé method can be obtained by computing the norm of the following relation:

$$\begin{aligned} G_{k+1} &= \mathrm{fl}\left(R_q\left(\frac{A}{m}\right)^{2^{k+1}}\right) - R_q\left(\frac{A}{m}\right)^{2^{k+1}} \\ &= \mathrm{fl}\left(R_q\left(\frac{A}{m}\right)^{2^{k}}\right)^2 + E_{k+1} - R_q\left(\frac{A}{m}\right)^{2^{k+1}} \\ &= G_k^2 + G_k R_q\left(\frac{A}{m}\right)^{2^{k+1}} + R_q\left(\frac{A}{m}\right)^{2^{k+1}} G_k + E_{k+1}, \end{aligned}$$

where $|E_{k+1}| < n\mathbf{u}|R_q(A/m)^{2^k}|^2$. If the matrix A is nonnegative, then we obtain

$$|G_{k+1}| < |G_k|^2 + |G_k| R_q\left(\frac{A}{m}\right)^{2^{k+1}} + R_q\left(\frac{A}{m}\right)^{2^{k+1}} |G_k| + n\mathbf{u} R_q\left(\frac{A}{m}\right)^{2^{k+1}},$$

and computing the 1-norm of this relation, we have

$$\|G_{k+1}\|_1 < \|G_k\|_1^2 + 2\|G_k\|_1 \left\| R_q\left(\frac{A}{m}\right)^{2^{k+1}} \right\|_1 + n\mathbf{u} \left\| R_q\left(\frac{A}{m}\right)^{2^{k+1}} \right\|_1 .$$

If we use such a relation, we obtain an approximate upper bound worse than the upper bound presented in Theorem 4.13(3).

(3) *The exponential of matrices $A = DBD^{-1}$, where D is diagonal and B is nonnegative.* Also if $A = DBD^{-1}, B$ nonnegative, the approximate upper bound presented in Theorem 4.13(3), is better than the upper bound introduced by Ward.

6. CONCLUSIONS

Theorem 4.13 summarizes the main results for the roundoff error introduced by the Padé method for computing e^A. We studied three special sets of matrices:

(1) A is essentially nonnegative;
(2) $A = DBD^{-1}, B$ essentially nonnegative, D diagonal;
(3) A is normal.

From the upper bounds presented in Theorem 4.13, we can conclude that the Padé algorithm is stable for the previous classes of matrices.

Note that in the upper bound to the roundoff error for computing the exponential of a normal matrix, the matrix order n is raised to the power $\frac{7}{2}$. We obtain this exponent because we use the 2-norm for computing the upper bound for

$$\frac{\|\mathrm{fl}\,(R_q(A/m)^m) - R_q(A/m)^m\|_1}{\|R_q(A/m)^m\|_1}.$$

It is our contention that, in practice, in this case we can use the upper bound

$$\begin{aligned}\frac{\|\mathrm{fl}\,(R_q(A/m)^m) - R_q(A/m)^m\|_1}{\|R_q(A/m)^m\|_1} &\dot{\leq} \mathbf{u}me^{1/2}[1+q(n+1)](1+e^{1/2}) \\ &\quad + \mathbf{u}n(m-1),\end{aligned}$$

neglecting the powers of n introduced by the passage to the 2-norm.

We can rewrite the upper bounds of Theorem 4.13 in a different form. In fact, the integer $m = 2^p$ is such that $0.25 \leq \|A\|_1/m < 0.5$, and so $m \leq 4\|A\|_1$; moreover, $4e^{1/2}(1+e^{1/2}) < 17.5$, and $e^{1/2}(1+e^{3/2}) < 9.04$.

Therefore, we can obtain the following upper bounds.

(1) If A is normal,

$$\begin{aligned}\frac{\|\mathrm{fl}(R_q(A/m)^m) - R_q(A/m)^m\|_1}{\|R_q(A/m)^m\|_1} &\dot{\leq} \mathbf{u}\|A\|_1 17.5[1+q(n+1)] + 4\mathbf{u}n\|A\|_1 \\ &= \mathbf{u}\|A\|_1 f_1(n,q).\end{aligned}$$

(2) If A is essentially nonnegative, or $A = DBD^{-1}, B$ essentially nonnegative, D diagonal,

$$\begin{aligned}\frac{\|\mathrm{fl}(R_q(A/m)^m) - R_q(A/m)^m\|_1}{\|R_q(A/m)^m\|_1} &\dot{\leq} \mathbf{u}\|A\|_1\{n + 9.04[1+q(n+1]\} \\ &= \mathbf{u}\|A\|_1 f_2(n,q).\end{aligned}$$

From Theorem 3.1 we have that the relative approximation error is less than or equal to $\mathbf{u}$ for very low values of q. In practice, we can then assume that $f_1(n,q)$ and $f_2(n,q)$ are growing as n and that both the previous upper bounds are $O(\mathbf{u}n\|A\|_1)$.

The numerical experiments that we ran on an IBM computer, model 3081, using relative single precision (2^{-20}) are in agreement with the previous conclusions.

We compute the matrix exponential of the following classes of matrices:

(1) nonnegative matrices;

(2) normal matrices;
(3) matrices of the form DAD^{-1}, where A is a nonnegative matrix and D is a diagonal matrix,

and we evaluate the error introduced by the Padé algorithm, assuming that the matrix obtained using the Padé method with double precision operations is a "good" approximation of the matrix exponential.

All the test matrices are real. Those of classes (1) and (3) are randomly generated, while the normal matrices are obtained by the formula QDQ^{-1}, where D is a diagonal matrix, $Q = I - 2vv^T$, v is a vector such that $\|v\|_2 = 1$, and I is the identity matrix; the matrix D and the vector v are constructed using a uniform random number generator.

From the numerical experiments, it turns out that, in practice, the relative roundoff error can be estimated by the upper bound $\mathbf{u}n\|A\|_1$.

Finally, we want to emphasize that in the class of the matrices diagonally similar to the essentially nonnegative matrices, we have examples of matrices presenting the well-known phenomen of the "hump" (see [12, 9]). The following two by two matrix is one of them:

$$A = \begin{pmatrix} -\beta & \alpha \\ 0 & -\beta \end{pmatrix}, \quad \alpha \geq 0,\ \beta \geq 0, \qquad e^{sA} = e^{-s\beta}\begin{pmatrix} 1 & s\alpha \\ 0 & 1 \end{pmatrix},$$
$$\|e^{sA}\|_1 = e^{-s\beta}(1 + s\alpha).$$

From the results of the paper we know that this hump has no influence on the final error. Moreover, we can observe that the hump is strictly related to the deviation from normality of the matrix from which we want to compute the exponential. These considerations suggest that for highly nonnormal matrices the presence of a cancellation during the squaring process may be the only real source of instability in the Padé method.

A possible alternative to the squaring [9, 12] is to translate the matrix A by a scalar factor λ such that the matrix $A + \lambda I$ has 1-norm less or equal to $\frac{1}{2}$, and then one can approximate e^A by $e^{-\lambda}R_{pq}(A + \lambda I)$. Corollary 4.8 insures that the result will be computed in a stable way.

It is possible to identify a subset of matrices for which such λ does exist. Let's denote

$$\rho_j = \sum_{i=1,\ i \neq j}^{n} |a_{ij}|.$$

Using the Gershgorin circle theorem, we have

$$\arg\min_{\lambda} \|A + \lambda I\|_1 = -\frac{1}{2}\Big(\max_j(a_{jj} + \rho_j) + \min_j(a_{jj} - \rho_j)\Big),$$

and the minimum value is equal to

$$\frac{1}{2}\Big(\max_j(a_{jj}+\rho_j)-\min_j(a_{jj}-\rho_j)\Big).$$

Therefore, for all the matrices for which the previous value is less or equal to $\frac{1}{2}$, the strategy of translation produces a stable algorithm.

REFERENCES

1 C. Fassino, Computation of matrix function, Ph.D. Thesis, Univ. of Pisa, 1993.

2 A. F. Fath, Evaluation of a matrix polynomial, *IEEE Trans. Automat. Control* AC-13:220–221 (1968).

3 G. H. Golub and C. Van Loan, *Matrix Computations*, 2nd ed., Johns Hopkins U. P., Baltimore, 1989.

4 J. L. Howland, Further ways to approximate the exponential of a matrix, *Linear and Multilinear Algebra* 14:121–129 (1983).

5 C. Moler and C. Van Loan, Nineteen dubious ways to compute the exponential of a matrix, *SIAM Rev.* 14:801–836 (1978).

6 L. F. Shampine and M. K. Gordon, *Computer Solution of Ordinary Differential Equations—The Initial Value Problem*, Freeman, San Francisco, 1975.

7 R. D. Skeel, Iterative refinement implies numerical stability for Gaussian elimination, *Math. Comp.* 35:817–832 (1980).

8 C. J. Standish, Truncated Taylor series approximation to the state transition matrix of a continuous parameter finite Markov chain, *Linear Algebra Appl.* 12:179–183 (1975).

9 C. Van Loan, On the limitation and application of Padé approximation to matrix exponential, in *Padé and Rational Approximation*, Academic, 1977, pp. 439–448.

10 ——, A note on the evaluation of matrix polynomials, *IEEE Trans. Automat. Control* AC-24:320–321 (1979).

11 R. S. Varga, *Matrix Iterative Analysis*, Prentice-Hall, Englewood Cliffs, N. J., 1962.

12 R. C. Ward, Numerical computation of the matrix exponential with accuracy estimate, *SIAM J. Numer. Anal.* 14:600–610 (1977).

13 G. Birkhoff and R. S. Varga, Reactor criticality and non-negative matrices, *J. Soc. Industr. Appl. Math.* 6:354–377 (1958).

Received 20 December 1993; final manuscript accepted 17 August 1994