and

$$Av_j = \lambda_j v_j, \qquad j = 1, \cdots, n.$$

These $n$ equations can be written

$$AV = VD.$$

where $D = \text{diag}(\lambda_1, \cdots, \lambda_n)$. The exponential of $D$ is trivial to compute assuming we have a satisfactory method for computing the exponential of a scalar:

$$e^{tD} = \text{diag}(e^{\lambda_1 t}, \cdots, e^{\lambda_n t}).$$

Since $V$ is nonsingular we have $e^{tA} = Ve^{tD}V^{-1}$.

In terms of the differential equation $\dot{x} = Ax$, the same eigenvector approach takes the following form. The initial condition is a combination of the eigenvectors,

$$x(0) = \sum_{j=1}^{n} \alpha_j v_j,$$

and the solution $x(t)$ is given by

$$x(t) = \sum_{j=0}^{n} \alpha_j e^{\lambda_j t} v_j.$$

Of course, the coefficients $\alpha_j$ are obtained by solving a set of linear equations $V\alpha = x(0)$.

The difficulty with this approach is not confluent eigenvalues per se. For example, the method works very well when $A$ is the identity matrix, which has an eigenvalue of the highest possible multiplicity. It also works well for any other symmetric matrix because the eigenvectors can be chosen orthogonal. If reliable subroutines such as TRED2 and TQL2 in EISPACK [113] are used, then the computed $v_j$ will be orthogonal to the full accuracy of the computer and the resulting algorithm for $e^{tA}$ has all the attributes we desire—except that it is limited to symmetric matrices.

The theoretical difficulty occurs when $A$ does not have a complete set of linearly independent eigenvectors and is thus defective. In this case there is no invertible matrix of eigenvectors $V$ and the algorithm breaks down. An example of a defective matrix is

$$\begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}.$$

A defective matrix has confluent eigenvalues but a matrix which has confluent eigenvalues need not be defective.

In practice, difficulties occur when $A$ is "nearly" defective. One way to make this precise is to use the condition number, $\text{cond}(V) = \|V\|\|V^{-1}\|$, of the matrix of eigenvectors. If $A$ is nearly (exactly) defective, then $\text{cond}(V)$ is large (infinite). Any errors in $A$, including roundoff errors in its computation and roundoff errors from the eigenvalue computation, may be magnified in the final result by $\text{cond}(V)$. Consequently, when $\text{cond}(V)$ is large, the computed $e^{tA}$ will most likely be inaccurate. For example, if

$$A = \begin{bmatrix} 1+\varepsilon & 1 \\ 0 & 1-\varepsilon \end{bmatrix},$$

then

$$V = \begin{bmatrix} 1 & -1 \\ 0 & 2\varepsilon \end{bmatrix},$$

$$D = \operatorname{diag}(1+\varepsilon, 1-\varepsilon),$$

and

$$\operatorname{cond}(V) = O\left(\frac{1}{\varepsilon}\right).$$

If $\varepsilon = 10^{-5}$ and IBM 370 short floating point arithmetic is used to compute the exponential from the formula $e^A = Ve^D V^{-1}$, we obtain

$$\begin{bmatrix} 2.718307 & 2.750000 \\ 0 & 2.718254 \end{bmatrix}.$$

Since the exact exponential to six decimals is

$$\begin{bmatrix} 2.718309 & 2.718282 \\ 0 & 2.718255 \end{bmatrix},$$

we see that the computed exponential has errors of order $10^5$ times the machine precision as conjectured.

One might feel that for this example $e^A$ might be particularly sensitive to perturbations in $A$. However, when we apply Theorem 3 in § 2 to this example, we find

$$\frac{\|e^{(A+E)} - e^A\|}{\|e^A\|} \leqq 4\|E\| e^{2\|E\|},$$

independent of $\varepsilon$. Certainly, $e^A$ is not overly sensitive to changes in $A$ and so Method 14 must be regarded as unstable.

Before we proceed to the next method it is interesting to note the connection between the use of eigenvectors and Method 9, Lagrange interpolation. When the eigenvalues are distinct the eigenvector approach can be expressed

$$e^{tA} = V \operatorname{diag}(e^{\lambda_i t}) V^{-1} = \sum_{j=1}^{n} e^{\lambda_j t} v_j y_j^T,$$

where $y_j^T$ is the $j$th row of $V^{-1}$. The Lagrange formula is

$$e^{tA} = \sum_{j=1}^{n} e^{\lambda_j t} A_j,$$

where

$$A_j = \prod_{\substack{k=1 \\ k \neq j}}^{n} \frac{(A - \lambda_k I)}{(\lambda_j - \lambda_k)}.$$

Because these two expressions hold for all $t$, the individual terms in the sum must be the same and so

$$A_j = v_j y_j^T.$$

This indicates that the $A_j$ are, in fact, rank one matrices obtained from the eigenvectors. Thus, the $O(n^4)$ work involved in the computation of the $A_j$ is totally unnecessary.

METHOD 15. TRIANGULAR SYSTEMS OF EIGENVECTORS. An improvement in both the efficiency and the reliability of the conventional eigenvector approach can be obtained when the eigenvectors are computed by the $QR$ algorithm [14]. Assume temporarily that although $A$ is not symmetric, all its eigenvalues happen to be real. The idea is to use EISPACK subroutines ORTHES and HQR2 to compute the eigenvalues and eigenvectors [113]. These subroutines produce an orthogonal matrix $Q$ and a triangular matrix $T$ so that

$$Q^TAQ = T.$$

Since $Q^{-1} = Q^T$, this is a similarity transformation and the desired eigenvalues occur on the diagonal of $T$. HQR2 next attempts to find the eigenvectors of $T$. This results in a matrix $R$ and a diagonal matrix $D$, which is simply the diagonal part of $T$, so that

$$TR = RD.$$

Finally, the eigenvectors of $A$ are obtained by a simple matrix multiplication $V = QR$.

The key observation is that $R$ is upper triangular. In other words, the ORTHES/HQR2 path in EISPACK computes the matrix of eigenvectors by first computing its "$QR$" factorization. HQR2 can be easily modified to remove the final multiplication of $Q$ and $R$. The availability of these two matrices has two advantages. First, the time required to find $V^{-1}$ or to solve systems involving $V$ is reduced. However, since this is a small fraction of the total time required, the improvement in efficiency is not very significant. A more important advantage is that cond $(V)$ = cond $(R)$ (in the 2-norm) and that the estimation of cond $(R)$ can be done reliably and efficiently.

The effect of admitting complex eigenvalues is that $R$ is not quite triangular, but has 2-by-2 blocks on its diagonal for each complex conjugate pair. Such a matrix is called quasi-triangular and we avoid complex arithmetic with minor inconvenience.

In summary, we suspect the following algorithm to be reliable:

(1) Given $A$, use ORTHES and a modified HQR2 to find orthogonal $Q$, diagonal $D$, and quasi-triangular $R$ so that

$$AQR = QRD.$$

(2) Given $x_0$, compute $y_0$ by solving

$$Ry_0 = Q^Tx_0.$$

Also estimate cond $(R)$ and hence the accuracy of $y_0$.

(3) If cond $(R)$ is too large, indicate that this algorithm cannot solve the problem and exit.

(4) Given $t$, compute $x(t)$ by

$$x(t) = Ve^{tD}y_0.$$

(If we want to compute the full exponential, then in Step 2 we solve $RY = Q^T$ for $Y$ and then use $e^{tA} = Ve^{tD}Y$ in Step 4.) It is important to note that the first three steps are independent of $t$, and that the fourth step, which requires relatively little work, can be repeated for many values of $t$.

We know there are examples where the exit is taken in Step 3 even though the *underlying problem* is not poorly conditioned implying that the algorithm is unstable.

Nevertheless, the algorithm is reliable insofar as cond $(R)$ enables us to assess the errors in the computed solution when that solution is found. It would be interesting to code this algorithm and compare it with Ward's scaling and squaring program for Method 3. In addition to comparing timings, the crucial question would be how often the exit in Step 3 is taken and how often Ward's program returns an unacceptably large error bound.

METHOD 16. JORDAN CANONICAL FORM. In principle, the problem posed by defective eigensystems can be solved by resorting to the Jordan canonical form (JCF). If

$$A = P[J_1 \oplus \cdots \oplus J_k]P^{-1}$$

is the JCF of $A$, then

$$e^{tA} = P[e^{tJ_1} \oplus \cdots \oplus e^{tJ_k}]P^{-1}.$$

The exponentials of the Jordan blocks $J_i$ can be given in closed form. For example, if

$$J_i = \begin{bmatrix} \lambda_i & 1 & 0 & 0 \\ 0 & \lambda_i & 1 & 0 \\ 0 & 0 & \lambda_i & 1 \\ 0 & 0 & 0 & \lambda_i \end{bmatrix},$$

then

$$e^{tJ_i} = e^{\lambda_i t}\begin{bmatrix} 1 & t & t^2/2! & t^3/3! \\ 0 & 1 & t & t^2/2! \\ 0 & 0 & 1 & t \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

The difficulty is that the JCF cannot be computed using floating point arithmetic. A single rounding error may cause some multiple eigenvalue to become distinct or vice versa altering the entire structure of $J$ and $P$. A related fact is that there is no a priori bound on cond $(P)$. For further discussion of the difficulties of computing the JCF, see the papers by Golub and Wilkinson [110] and Kågstrom and Ruhe [111].

METHOD 17. SCHUR. The Schur decomposition

$$A = QTQ^T$$

with orthogonal $Q$ and triangular $T$ exists if $A$ has real eigenvalues. If $A$ has complex eigenvalues, then it is necessary to allow 2-by-2 blocks on the diagonal of $T$ or to make $Q$ and $T$ complex (and replace $Q^T$ with $Q^*$). The Schur decomposition can be computed reliably and quite efficiently by ORTHES and a short-ended version of HQR2. The required modifications are discussed in the EISPACK guide [113].

Once the Schur decomposition is available,

$$e^{tA} = Q\,e^{tT}Q^T.$$

The only delicate part is the computation of $e^{tT}$ where $T$ is a triangular or quasi-triangular matrix. Note that the eigenvectors of $A$ are not required.

Computing functions or triangular matrices is the subject of a recent paper by Parlett [112]. If $T$ is upper triangular with diagonal elements $\lambda_1, \cdots, \lambda_n$, then it is clear that $e^{tT}$ is upper triangular with diagonal elements $e^{\lambda_1 t}, \cdots, e^{\lambda_n t}$. Parlett shows how to compute the off-diagonal elements of $e^{tT}$ recursively from divided differences of the $e^{\lambda_i t}$. The example in § 1 illustrates the 2-by-2 case.

Again, the difficulty is magnification of roundoff error caused by nearly confluent eigenvalues $\lambda_i$. As a step towards handling this problem, Parlett describes a generalization of his algorithm applicable to block upper triangular matrices. The diagonal blocks are determined by clusters of nearby eigenvalues. The confluence problems do not disappear, but they are confined to the diagonal blocks where special techniques can be applied.

METHOD 18. BLOCK DIAGONAL. All methods which involve decompositions of the form

$$A = SBS^{-1}$$

involve two conflicting objectives:

(1) Make $B$ close to diagonal so that $e^{tB}$ is easy to compute.

(2) Make $S$ well conditioned so that errors are not magnified.

The Jordan canonical form places all the emphasis on the first objective, while the Schur decomposition places most of the emphasis on the second. (We would regard the decomposition with $S = I$ and $B = A$ as placing even more emphasis on the second objective.)

The block diagonal method is a compromise between these two extremes. The idea is to use a nonorthogonal, but well conditioned, $S$ to produce a $B$ which is triangular and block diagonal as illistrated in Fig. 2.

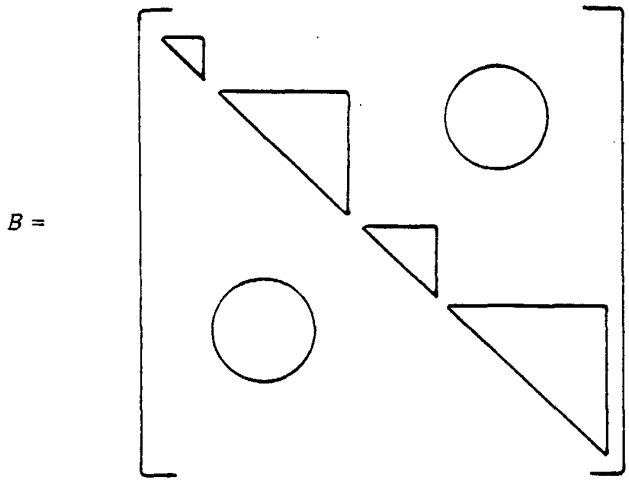


FIG. 2. *Triangular block diagonal form.*

Each block in $B$ involves a cluster of nearly confluent eigenvalues. The number in each cluster (the size of each block) is to be made as small as possible while maintaining some prescribed upper bound for cond $(S)$, such as cond $(S) < 100$. The choice of the bound 100 implies roughly that at most 2 significant decimal figures will be lost because of rounding errors when $e^{tA}$ is obtained from $e^{tB}$ via $e^{tA} = Se^{tB}S^{-1}$. A larger bound would mean the loss of more figures while a smaller bound would mean more computer time—both for the factorization itself and for the evaluation of $e^{tB}$.

In practice, we would expect almost all the blocks to be 1-by-1 or 2-by-2 and the resulting computation of $e^{tB}$ to be very fast. The bound on cond $(S)$ will mean that it is occasionally necessary to have larger blocks in $B$, but it will insure against excessive loss of accuracy from confluent eigenvalues.

G. W. Stewart has pointed out that the grouping of the eigenvalues into clusters and the resulting block structure of $B$ is not merely for increased speed. There can be an important improvement in accuracy. Stewart suggests expressing each block $B_j$ in the form

$$B_j = \gamma_j I + E_j$$

where $\gamma_j$ is the average value of the eigenvalues in the $j$th cluster. If the grouping has been done properly, the matrices $E_j$ should then be nearly nilpotent in the sense that $E_j^k$ will rapidly approach zero as $k$ increases. Since $E_j$ is triangular, this will certainly be true if the diagonal part of $E_j$ is small, that is, if all the eigenvalues in the cluster are close together. But it will also be true in another important case. If

$$E_j = \begin{bmatrix} \sqrt{\varepsilon} & 1 \\ 0 & -\sqrt{\varepsilon} \end{bmatrix},$$

where $\varepsilon$ is the computer rounding unit, then

$$E_j^2 = \begin{bmatrix} \varepsilon & 0 \\ 0 & \varepsilon \end{bmatrix}$$

can be regarded as negligible. The $\pm\sqrt{\varepsilon}$ perturbations are typical when a double, defective eigenvalue is computed with, say, HQR2.

The fact that $E_j$ is nearly nilpotent means that $e^{tB_j}$ can be found rapidly and accurately from

$$e^{tB_j} = e^{\gamma_j t} e^{tE_j};$$

computing $e^{tE_j}$ by a few terms of the Taylor series.

Several researchers, including Parlett, Ruhe, and Stewart, are currently developing computer programs based on some of these ideas. The most difficult detail is the proper choice of the eigenvalue clustering. It is also important for program efficiency to avoid complex arithmetic as much as possible. When fully developed, these programs will be fairly long and complicated but they may come close to meeting our other criteria for satisfactory methods.

Most of the computational cost lies in obtaining the basic Schur decomposition. Although this cost varies somewhat from matrix to matrix because of the iterative nature of the $QR$ algorithm, a good average figure is $15\,n^3$ flops, including the further reduction to block diagonal form. Again we emphasize that the reduction is independent of $t$. Once the decomposition is obtained, the calculation of $e^{tA}$ requires about $2\,n^3$ flops for each $t$. If we require only $x(t) = e^{tA}x_0$ for various $t$, the equation $Sy = x_0$ should be solved once at a cost of $n^3/3$ flops, and then each $x(t)$ can be obtained with $n^2$ flops.

These are rough estimates. There will be differences between programs based on the Schur decomposition and those which work with the block diagonal form, but the timings should be similar because Parlett's algorithm for the exponential is very fast.

**7. Splitting methods.** A most aggravating, yet interesting, property of the matrix exponential is that the familiar additive law fails unless we have commutivity:

$$e^{tB}\,e^{tC} = e^{t(B+C)} \Leftrightarrow BC = CB.$$

Nevertheless, the exponentials of $B$ and $C$ are related to that of $B + C$, for example,

by the Trotter product formula [30]:

$$e^{B+C} = \lim_{m\to\infty} (e^{B/m} e^{C/m})^m.$$

METHOD 19. SPLITTING. Our colleagues M. Gunzburger and D. Gottleib suggested that the Trotter result be used to approximate $e^A$ by splitting $A$ into $B+C$ and then using the approximation

$$e^A \simeq (e^{B/m} e^{C/m})^m.$$

This approach to computing $e^A$ is of potential interest when the exponentials of $B$ and $C$ can be accurately and efficiently computed. For example, if $B=(A+A^T)/2$ and $C=(A-A^T)/2$ then $e^B$ and $e^C$ can be effectively computed by the methods of § 5. For this choice we show in Appendix 2 that

$$\|e^A - (e^{B/m} e^{C/m})^m\| \leqq \frac{\|[A^T, A]\|}{4m} e^{\mu(A)}, \tag{7.1}$$

where $\mu(A)$ is the log norm of $A$ as defined in § 2. In the following algorithm, this inequality is used to determine the parameter $m$.

(a) Set $B=(A+A^T)/2$ and $C=(A-A^T)/2$. Compute the factorization $B = Q \operatorname{diag}(\mu_i) Q^T$ $(Q^TQ=I)$ using TRED2 and TQL2 [113]. Variations of these programs can be used to compute the factorization $C=UDU^T$ where $U^TU=I$ and $D$ is the direct sum of zero matrices and real 2-by-2 blocks of the form

$$\begin{bmatrix} 0 & a \\ -a & 0 \end{bmatrix}$$

corresponding to eigenvalues $\pm ia$.

(b) Determine $m=2^j$ such that the upper bound in (7.1) is less than some prescribed tolerance. Recall that $\mu(A)$ is the most positive eigenvalue of $B$ and that this quantity is known as a result of step (a).

(c) Compute $X = Q \operatorname{diag}(e^{\mu_i/m}) Q^T$ and $Y = U e^{D/m} U^T$. In the latter computation, one uses the fact that

$$\exp\begin{bmatrix} 0 & a/m \\ -a/m & 0 \end{bmatrix} = \begin{bmatrix} \cos(a/m) & \sin(a/m) \\ -\sin(a/m) & \cos(a/m) \end{bmatrix}$$

(d) Compute the approximation, $(XY)^{2^j}$, to $e^A$ by repeated squaring.

If we assume $5n^3$ flops for each of the eigenvalue decompositions in (a), then the overall process outlined above requires about $(13+j)n^3$ flops. It is difficult to assess the relative efficiency of this splitting method because it depends strongly on the scalars $\|[A^T, A]\|$ and $\mu(A)$ and these quantities have not arisen in connection with any of our previous eighteen methods. On the basis of truncation error bounds, however, it would seem that this technique would be much less efficient than Method 3 (scaling and squaring) unless $\mu(A)$ were negative and $\|[A^T, A]\|$ much less than $\|A\|$.

Accuracy depends on the rounding errors which arise in (d) as a result of the repeated squaring. The remarks about repeated squaring in Method 3 apply also here: there may be severe cancellation but whether or not this only occurs in sensitive $e^A$ problems is unknown.

For a general splitting $A = B + C$, we can determine $m$ from the inequality

$$\|e^A - (e^{B/m} e^{C/m})^m\| \leqq \frac{\|[B, C]\|}{2m} e^{\|B\|+\|C\|}, \tag{7.2}$$

which we establish in Appendix 2.

To illustrate, suppose $A$ has companion form

$$A = \begin{bmatrix} 0 & 1 & & 0 \cdots 0 \\ \vdots & & \ddots & \vdots \\ & & & 1 \\ c_0 & c_1 & \cdots & c_{n-1} \end{bmatrix}.$$

If

$$B = \begin{bmatrix} 0 & I_{n-1} \\ 0 & 0 \end{bmatrix}$$

and $C = e_n c^T$ where $c^T = (c_0, \cdots, c_{n-1})$ and $e_n^T = (0, 0, \cdots, 0, 1)$, then

$$e^{B/m} = \sum_{k=0}^{n-1} \left[\frac{B}{m}\right]^k \frac{1}{k!}$$

and

$$e^{C/m} = I + \frac{e^{c_{n-1}/m} - 1}{c_{n-1}} e_n c^T.$$

Notice that the computation of these scaled exponentials require only $O(n^2)$ flops. Since $\|B\| = 1$, $\|C\| = \|c\|$, and $\|[B, C]\| \leqq 2\|c\|$, (7.2) becomes

$$\|e^A - (e^{B/m} e^{C/m})^m\| \leqq \frac{e^{1+\|c\|}\|c\|}{m}.$$

The parameter $m$ can be determined from this inequality.

**8. Conclusions.** A section called "conclusions" must deal with the obvious question: Which method is best? Answering that question is very risky. We don't know enough about the sensitivity of the original problem, or about the detailed performance of careful implementations of various methods to make any firm conclusions. Furthermore, by the time this paper appears in the open literature, any given conclusion might well have to be modified.

We have considered five general classes of methods. What we have called polynomial methods are not really in the competition for "best". Some of them require the characteristic polynomial and so are appropriate only for certain special problems and others have the same stability difficulties as matrix decomposition methods but are much less efficient. The approaches we have outlined under splitting methods are largely speculative and untried and probably only of interest in special settings. This leaves three classes in the running.

The only generally competitive series method is Method 3, scaling and squaring. Ward's program implementing this method is certainly among the best currently available. The program may fail, but at least it tells you when it does. We don't know yet whether or not such failures usually result from the inherent sensitivity of the

problem or from the instability of the algorithm. The method basically computes $e^A$ for a single matrix $A$. To compute $e^{tA}$ for $p$ arbitrary values of $t$ requires about $p$ times as much work. The amount of work is $O(n^3)$, even for the vector problem $e^{tA}x_0$. The coefficient of $n^3$ increases as $\|A\|$ increases.

Specializations of o.d.e. methods for the $e^A$ problem have not yet been implemented. The best method would appear to involve a variable order, variable step difference scheme. We suspect it would be stable and reliable but expensive. Its best showing on efficiency would be for the vector problem $e^{tA}x_0$ with many values of $t$ since the amount of work is only $O(n^2)$. It would also work quite well for vector problems involving a large sparse $A$ since no "nonsparse" approximation to the exponential would be explicitly required.

The best programs using matrix decomposition methods are just now being written. They start with the Schur decomposition and include some sort of eigenvalue clustering. There are variants which involve further reduction to a block form. In all cases the initial decomposition costs $O(n^3)$ steps and is independent of $t$ and $\|A\|$. After that, the work involved in using the decomposition to compute $e^{tA}x_0$ for different $t$ and $x_0$ is only a small multiple of $n^2$.

Thus, we see perhaps three or four candidates for "best" method. The choice will depend upon the details of implementation and upon the particular problem being solved.

**Appendix 1. Inverse error analysis of Padé matrix approximation.**

LEMMA 1. *If* $\|H\| < 1$, *then* $\log(I+H)$ *exists and*

$$\|\log(I+H)\| \leqq \frac{\|H\|}{1-\|H\|}.$$

*Proof.* If $\|H\| < 1$ then $\log(I+H) = \sum_{k=1}^{\infty} (-1)^{k+1}(H^k/k)$ and so

$$\|\log(I+H)\| \leqq \sum_{k=1}^{\infty} \frac{\|H\|^k}{k} \leqq \|H\| \sum_{k=0}^{\infty} \|H\|^k = \frac{\|H\|}{1-\|H\|}.$$

LEMMA 2. *If* $\|A\| \leqq \frac{1}{2}$ *and* $p > 0$, *then* $\|D_{pq}(A)^{-1}\| \leqq (q+p)/p$.

*Proof.* From the definition of $D_{pq}(A)$ in § 3, $D_{pq}(A) = I + F$ where

$$F = \sum_{j=1}^{q} \frac{(p+q-j)!q!}{(p+q)!(q-j)!} \frac{(-A)^j}{j!}.$$

Using the fact that

$$\frac{(p+q-j)!q!}{(p+q)!(q-j)!} \leqq \left[\frac{q}{p+q}\right]^j$$

we find

$$\|F\| \leqq \sum_{j=1}^{q} \left[\frac{q}{p+q}\|A\|\right]^j \frac{1}{j!} \leqq \frac{q}{p+q}\|A\|(e-1) \leqq \frac{q}{p+q}$$

and so $\|D_{pq}(A)^{-1}\| = \|(I+F)^{-1}\| \leqq 1/(1-\|F\|) \leqq (q+p)/p$.

LEMMA 3. *If* $\|A\| \leqq \frac{1}{2}$, $q \leqq p$, *and* $p \geqq 1$, *then* $R_{pq}(A) = e^{A+F}$ *where*

$$\|F\| \leqq 8\|A\|^{p+q+1} \frac{p!q!}{(p+q)!(p+q+1)!}.$$

*Proof.* From the remainder theorem for Padé approximants [71],

$$R_{pq}(A)=e^{A}-\frac{(-1)^{q}}{(p+q)!}A^{p+q+1}D_{pq}(A)^{-1}\int_{0}^{1}e^{(1-u)A}u^{p}(1-u)^{q}\,du,$$

and so $e^{-A}R_{pq}(A)=I+H$ where

$$H=\frac{(-1)^{q+1}}{(p+q)!}A^{p+q+1}D_{pq}(A)^{-1}\int_{0}^{1}e^{-uA}u^{p}(1-u)^{q}\,du.$$

By taking norms, using Lemma 2, and noting that $(p+q)/p\,e^{s}\leqq 4$ we obtain

$$\|H\|\leqq\frac{1}{(p+q)!}\|A\|^{p+q+1}\frac{p+q}{p}\int_{0}^{1}e^{s}u^{p}(1-u)^{q}\,du$$

$$\leqq 4\|A\|^{p+q+1}\frac{p!q!}{(p+q)!(p+q+1)!}.$$

With the assumption $\|A\|\leqq\frac{1}{2}$ it is possible to show that for all admissable $p$ and $q$, $\|H\|\leqq\frac{1}{2}$ and so from Lemma 1,

$$\|\log(I+H)\|\leqq\frac{\|H\|}{1-\|H\|}\leqq 8\|A\|^{p+q+1}\frac{p!q!}{(p+q)!(p+q+1)!}.$$

Setting $F=\log(I+H)$, we see that $e^{-A}R_{pq}(A)=I+H=e^{F}$. The lemma now follows because $A$ and $F$ commute implying $R_{pq}(A)=e^{A}e^{F}=e^{A+F}$.

LEMMA 4. *If* $\|A\|\leqq\frac{1}{2}$ *then* $R_{pq}(A)=e^{A+F}$ *where*

$$\|F\|\leqq 8\|A\|^{p+q+1}\frac{p!q!}{(p+q)!(p+q+1)!}.$$

*Proof.* The case $p\geqq q$, $p\geqq 1$ is covered by Lemma 1. If $p+q=0$, then $F=-A$ and the above inequality holds. Finally, consider the case $q>p$, $q\geqq 1$. From Lemma 3, $R_{qp}(-A)=e^{-A+F}$ where $F$ satisfies the above bound. The lemma now follows because $\|-F\|=\|F\|$ and $R_{pq}(A)=[R_{qp}(-A)]^{-1}=[e^{-A+F}]^{-1}=e^{A-F}$.

THEOREM A.1. *If* $\|A\|/2^{i}\leqq\frac{1}{2}$, *then* $[R_{pq}(A/2^{i})]^{2^{i}}=e^{A+E}$ *where*

$$\frac{\|E\|}{\|A\|}\leqq 8\left(\frac{\|A\|}{2^{i}}\right)^{p+q}\frac{p!q!}{(p+q)!(p+q+1)!}\leqq\left(\frac{1}{2}\right)^{p+q-3}\frac{p!q!}{(p+q)!(p+q+1)!}.$$

*Proof.* From Lemma 4, $R_{pq}(A/2^{i})=e^{A+F}$ where

$$\|F\|\leqq 8\left[\frac{\|A\|}{2^{i}}\right]^{p+q+1}\frac{p!q!}{(p+q)!(p+q+1)!}.$$

The theorem follows by noting that if $E=2^{i}F$, then

$$\left[R_{pq}\left(\frac{A}{2^{i}}\right)\right]^{2^{i}}=[e^{A/2^{i}+F}]^{2^{i}}=e^{A+E}.$$

COROLLARY 1. *If* $\|A\|/2^{i}\leqq\frac{1}{2}$, *then* $[T_{k}(A/2^{i})]^{2^{i}}=e^{A+E}$ *where*

$$\frac{\|E\|}{\|A\|}\leqq 8\left(\frac{\|A\|}{2^{i}}\right)^{k}\cdot\frac{1}{k+1}\leqq\left(\frac{1}{2}\right)^{k-3}\frac{1}{k+1}.$$

COROLLARY 2. *If* $\|A\|/2^i \leqq \frac{1}{2}$, *then* $[R_{qq}(A/2^i)]^{2^i} = e^{A+E}$, *where*

$$\frac{\|E\|}{\|A\|} \leqq 8\left(\frac{\|A\|}{2^i}\right)^{2q} \cdot \frac{(q!)^2}{(2q)!(2q+1)!} \leqq \left(\frac{1}{2}\right)^{2q-3} \frac{(q!)^2}{(2q)!(2q+1)!}.$$

**Appendix 2. Accuracy of splitting techniques.** In this appendix we derive the inequalities (7.1) and (7.2). We assume throughout that $A$ is an $n$-by-$n$ matrix and that

$$A = B + C.$$

It is convenient to define the matrices

$$S_m = e^{A/m},$$

and

$$T_m = e^{B/m} e^{C/m},$$

where $m$ is a positive integer. Our goal is to bound $\|S_m^m - T_m^m\|$. To this end we shall have to exploit the following properties of the log norm $\mu(A)$ defined in § 2:

$$\text{(i)} \quad \|e^{tA}\| \leqq e^{\mu(A)t} \qquad (t \geqq 0)$$

$$\text{(ii)} \quad \mu(A) \leqq \|A\|$$

$$\text{(iii)} \quad \mu(B+C) \leqq \mu(B) + \|C\|.$$

These and other results concerning log norms are discussed in references [35]–[42].

LEMMA 1. *If* $\Theta \geqq \max\{\mu(A), \mu(B)+\mu(C)\}$ *then*

$$\|S_m^m - T_m^m\| \leqq m\, e^{\Theta(m-1)/m} \|S_m - T_m\|.$$

*Proof.* Following Reed and Simon [11] we have

$$S_m^m - T_m^m = \sum_{k=0}^{m-1} S_m^k (S_m - T_m) T_m^{m-1-k}.$$

Using log norm property (i) it is easy to show that both $\|S_m\|$ and $\|T_m\|$ are bounded above by $e^{\Theta/m}$ and thus

$$\|S_m^m - T_m^m\| \leqq \sum_{k=0}^{m-1} \|S_m\|^k \|S_m - T_m\| \|T_m\|^{m-1-k}$$

$$\leqq \|S_m - T_m\| \sum_{k=0}^{m-1} e^{\Theta k/m} e^{\Theta(m-1-k)/m},$$

from which the lemma immediately follows.

In Lemmas 2 and 3 we shall make use of the notation

$$F(t)\Big|_{t=t_0}^{t=t_1} = F(t_1) - F(t_0),$$

where $F(t)$ is a matrix whose entries are functions of $t$.

LEMMA 2.

$$T_m - S_m = \int_0^1 e^{tB/m} \left[ e^{(1-t)A/m}, \frac{1}{m} C \right] e^{tC/m}\, dt.$$

*Proof.* We have $T_m - S_m = e^{tB/m} e^{(1-t)A/m} e^{tC/m} \Big|_{t=0}^{t=1}$ and thus

$$T_m - S_m = \int_0^1 \left\{ \frac{d}{dt} [e^{tB/m} e^{(1-t)A/m} e^{tC/m}] \right\} dt.$$

The lemma follows since

$$\frac{d}{dt} [e^{tB/m} e^{(1-t)A/m} e^{tC/m}] = e^{tB/m} \left[ e^{(1-t)A/m}, \frac{1}{m} C \right] e^{tC/m}.$$

LEMMA 3. *If $X$ and $Y$ are matrices then*

$$|||[e^X, Y]||| \leqq e^{\mu(X)} |||[X, Y]|||.$$

*Proof.* We have $[e^X, Y] = e^{tX} Y e^{(1-t)X} \Big|_{t=0}^{t=1}$ and thus

$$[e^X, Y] = \int_0^1 \left\{ \frac{d}{dt} [e^{tX} Y e^{(1-t)X}] \right\} dt.$$

Since $d/dt[e^{tX} Y e^{(1-t)X}] = e^{tX}[X, Y] e^{(1-t)X}$ we get

$$|||[e^X, Y]||| \leqq \int_0^1 \|e^{tX}\| |||[X, Y]||| \|e^{(1-t)X}\| \, dt$$

$$\leqq |||[X, Y]||| \int_0^1 e^{\mu(X)t} e^{\mu(X)(1-t)} \, dt$$

from which the lemma immediately follows.

THEOREM A.2. *If $\Theta \geqq \max \{\mu(A), \mu(B) + \mu(C)\}$, then*

$$\|S_m^m - T_m^m\| \leqq \frac{1}{2m} e^{\Theta} |||[B, C]|||.$$

*Proof.* If $0 \leqq t \leqq 1$ then an application of Lemma 3 with $X \equiv (1-t)A/m$ and $Y \equiv C/m$ yields

$$|||[e^{(1-t)A/m}, C/m]||| \leqq e^{\mu(A)(1-t)/m} |||[(1-t)A/m, C/m]|||$$

$$\leqq e^{\Theta(1-t)/m} \frac{(1-t)}{m^2} |||[B, C]|||.$$

By coupling this inequality with Lemma 2 we can bound $\|T_m - S_m\|$:

$$\|T_m - S_m\| \leqq \int_0^1 \|e^{tB/m}\| |||[e^{(1-t)A/m}, C/m]||| \|e^{tC/m}\| \, dt$$

$$\leqq \int_0^1 e^{\mu(B)t/m} e^{\Theta(1-t)/m} \frac{(1-t)}{m^2} |||[B, C]||| \, e^{\mu(C)t/m} \, dt$$

$$\leqq \frac{1}{2} e^{\Theta/m} \frac{|||[B, C]|||}{m^2}.$$

The theorem follows by combining this result with Lemma 1.

COROLLARY 1. *If $B = (A + A^*)/2$ and $C = (A - A^*)/2$ then*

$$\|S_m^m - T_m^m\| \leqq \frac{1}{4m} e^{\mu(A)} |||[A^*, A]|||.$$

*Proof.* Since $\mu(A)=\mu(B)$ and $\mu(C)=0$, we can set $\Theta=\mu(A)$. The corollary is established by noting that $[B, C]=\frac{1}{2}[A^*, A]$.

COROLLARY 2.

$$\|S_m^m - T_m^m\| \leqq \frac{1}{2m} e^{\mu(B)+\|C\|}\|[B, C]\| \leqq \frac{1}{2m} e^{\|B\|+\|C\|}\|[B, C]\|.$$

*Proof.* $\max\{\mu(A), \mu(B)+\mu(C)\} \leqq \mu(B)+\|C\| \leqq \|B\|+\|C\|$.

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