On Asymptotic Expansions for Functions of Matrix Argument

YUDELL L. LUKE* AND G. P. BARKER

University of Missouri, Kansas City, Missouri 64110

Communicated by Oved Shisha

Received July 18, 1977

In a previous paper [1], J. J. Williams and R. Wong studied the problem of the title and its application to the extension of the scalar form of Watson's lemma. In their work, a key assumption is that the matrix is normal. In the present paper, the problem is studied without this assumption.

In Section I, we present a definition of asymptotic expansion for functions of matrix argument and give conditions when f(z), z a scalar, has an asymptotic expansion with z replaced by a matrix A. In Section II, the analog of Watson's lemma is treated. Some results concerning the asymptotic but divergent series expansion of the exponential integral are reviewed in Section II. The analogous matrix expansion also diverges. This suggests use of rational approximations, say of the Padé type, and Chebyshev expansions. This is also treated in Section III. Finally, the ideas are illustrated with numerical examples in Section IV.

I. DEFINITION OF EXPANSIONS FOR FUNCTIONS OF MATRIX ARGUMENT

Let A be an $n \times n$ matrix with complex entries, $A = (a_{ij})$.

DEFINITION. We say that the formal series

$$\sum_{k=0}^{\infty} b_k A^{-k} \tag{1}$$

is an asymptotic expansion of the function f(A), where f(z) is defined and analytic on the spectrum $\sigma(A)$, if for all $N \ge n$,

$$||f(A) - \sum_{k=0}^{N} b_k A^{-k}|| = o(||A^{-N}||)$$
 (2)

^{*} The research work of this author was sponsored by the Air Force Office of Scientific Research under Grant 73-2520.

as $||A^{-1}|| \to 0$. In this event, we write

$$f(A) \sim \sum_{k=0}^{\infty} b_k A^{-k}, \quad ||A^{-1}|| \to 0.$$
 (3)

Here the norm is understood to be a least upper bound norm on the matrices of complex numbers.

Let $J \equiv J(A)$ be the Jordan normal form of A. Then there exists a non-singular matrix P such that $P^{-1}AP = J$ and clearly

$$P^{-1}A^nP = J^n$$
, n a positive integer or zero. (4)

We will have need for the condition number of P which is defined as

$$n(P) = ||P|| ||P^{-1}||. (5)$$

The following assumptions are made on the spectrum of A, $\sigma(A)$, and n(P) respectively.

$$\sigma(A) \subset \{\lambda; \ \lambda \neq 0, \ |\arg(\lambda - \theta)| < \Delta\},\$$

$$0 < \Delta < \pi/2, \qquad 0 < \theta < 2\pi.$$
(6)

$$n(P)$$
 is bounded as $||A^{-1}|| \rightarrow 0$. (7)

We prove the following

THEOREM 1. Let f(z) be analytic in the domain $|\arg(z-\theta)| < \Delta$ and let f(z) have the asymptotic series expansion

$$f(z) \sim \sum_{k=0}^{\infty} b_k z^{-k}, \qquad |z| \to \infty$$
 (8)

with arg z restricted as above. Let A be a matrix satisfying the conditions (6) and (7). Then

$$f(A) \sim \sum_{k=0}^{\infty} b_k A^{-k}, \quad ||A^{-1}|| \to 0.$$
 (9)

Proof. Let $N \ge n$. Since matrix norms are equivalent, we choose the row-sum norm

$$||A|| = \max_{1 \le i \le n} \left\{ \sum_{i=1}^{n} |a_{ij}| \right\}.$$
 (10)

It is sufficient to prove that

$$f(J) \sim \sum_{k=0}^{\infty} b_k J^{-k},\tag{11}$$

for if (11) is true, we have

$$|| f(A) - \sum_{k=0}^{N} b_k A^{-k} || = || P \left\{ f(J) - \sum_{k=0}^{N} b_k J^{-k} \right\} P^{-1} ||$$

$$\leq n(P) || f(J) - \sum_{k=0}^{N} b_k J^{-k} ||$$

$$\leq \epsilon n(P) || J^{-N} || \leq \epsilon \{ n(P) \}^2 || A^{-N} ||.$$

$$(12)$$

Since ϵ can be made arbitrarily small and n(P) is bounded, the theorem follows once we have established (11). To this end, let B be a block of order m of the Jordan normal form of A which we write as

$$B = \begin{pmatrix} \lambda & 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & \lambda & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \lambda & 1 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \lambda & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \lambda & 1 \\ 0 & 0 & 0 & 0 & \cdots & 0 & \lambda \end{pmatrix}. \tag{13}$$

Then a straightforward computation shows that for any f(z),

$$f(B) = \begin{bmatrix} f(\lambda) & f'(\lambda) & \frac{1}{2!} f''(\lambda) & \cdots & \frac{1}{(m-1)!} f^{(m-1)}(\lambda) \\ 0 & f(\lambda) & f'(\lambda) & \cdots & \frac{1}{(m-2)!} f^{(m-2)}(\lambda) \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & f(\lambda) \end{bmatrix}$$
(14)

If

$$g(z) = \sum_{k=0}^{\infty} c_k z^{-k},$$
 (15)

$$g^{(r)}(z) = (-1)^r \sum_{k=0}^{\infty} \{(k+r-1)!/(k-1)!\} c_k z^{-k-r}.$$
 (16)

Thus with

$$g_N(z) = \sum_{k=0}^{N} c_k z^{-k}, \tag{17}$$

$$\sum_{k=0}^{N} b_{k} B^{-k} = \begin{bmatrix} g_{N}(B) & g_{N}'(B) & \cdots & \frac{1}{(m-1)!} g_{N}^{(m-1)}(B) \\ 0 & g_{N}(B) & \cdots & \frac{1}{(m-2)!} g_{N}^{(m-2)}(B) \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 0, & \cdots & g_{N}(B) \end{bmatrix}.$$
(18)

In view of (8), we have

$$\left| \frac{f'(\lambda)}{r!} - \frac{(-1)^r}{r!} \sum_{k=0}^N \frac{(k+r-1)! \ b_k \lambda^{-k-r}}{(k-1)!} \right| = o(|\lambda|^{-N}). \tag{19}$$

So, from (10),

$$\left\| f(B) - \sum_{k=0}^{N} b_k B^{-k} \right\|$$

$$\leq \sum_{r=0}^{m-1} \left| f^{(r)}(\lambda) - \frac{(-1)^{r-1}}{(r-1)!} \sum_{k=0}^{N} \frac{(k+r-1)! b_k z^{-k-r+1}}{(k-1)!} \right|. \quad (20)$$

But

$$||B^{-N}|| = \sum_{r=0}^{m} \frac{N!}{(N-r)!} |\lambda^{-N-r}| = |\lambda^{-N}| + o(|\lambda^{-N}|).$$
 (21)

Thus

$$||f(B) - \sum_{k=0}^{N} b_k B^{-k}|| = o(||B^{-N}||).$$
 (22)

That is,

$$f(B) \sim \sum_{k=0}^{\infty} b_k B^{-k}, \tag{23}$$

and the statement (9) follows.

COROLLARY 1. If A is a normal matrix satisfying (6), and if f(z) is as in the above theorem, then

$$f(A) \sim \sum_{k=0}^{\infty} b_k A^{-k}.$$
 (24)

Proof. Take the spectral norm $\mu(A)$ subordinate to the l_2 norm where $l_2(x) = (x^*x)^{1/2}$. Then A is a unitarily equivalent to a diagonal matrix. We can take P in the definition of J, see [4], to be unitary. Then P^{-1} is also unitary and n(P) = 1.

COROLLARY 2. If $A = \alpha C$ where α is a positive scalar and C is diagonalizable, and if f(z) satisfies the conditions for the above theorem, then

$$f(\alpha A) \sim \sum_{k=0}^{\infty} b_k \alpha^k A^{-k} \quad as \quad \alpha \to \infty.$$
 (25)

II. WATSON'S LEMMA

In this section we treat the analog of Watson's lemma for functions of matrix argument. Rather than give a detailed proof of same, we state a result of J. J. Williams and R. Wong [1] for closed operators and show that our system of matrices satisfy the hypotheses of their theorem.

It is convenient to first state Watson's lemma in the scalar case. Let f(t) be locally integrable on $[0, \infty)$, and let

$$g(z) = \int_0^\infty e^{-zt} f(t) dt$$
 (26)

whenever the integral on the right converges. Let

$$f(t) = \sum_{k=1}^{\infty} a_k t^{k/r-1}, \qquad |t| \leqslant c + \delta, \tag{27}$$

where r, c and δ are positive, and let there exist positive constants N and b independent of t such that

$$|f(t)| \leqslant Ne^{bt}, \qquad t \geqslant c. \tag{28}$$

Then

$$g(z) \sim \sum_{k=1}^{\infty} a_k \Gamma(k/r) z^{-k/r},$$

$$|z| \to \infty, \quad |\arg z| \leqslant \pi/2 - \Delta, \quad \Delta > 0.$$
(29)

Consider a closed operator A which satisfies the following two conditions on the spectrum $\sigma(A)$.

There exists a positive Δ such that

$$\sigma(A) \subseteq \{\lambda \in \mathbb{C} : \lambda \neq 0 \text{ and } | \arg \lambda | \leqslant \pi/2 - \Delta \}.$$
 (30)

Let $\omega(A) = \inf\{\text{Re } \lambda : \lambda \in \sigma(A)\}$. There exists M > 0 and $0 < \omega_1 \le \omega(A)$ such that for any positive integer m,

$$||R_{\lambda}(A)^{m}|| \leq M/(\omega_{1}-\lambda)^{m}, \qquad \omega_{1} > \lambda > 0.$$

$$R_{\lambda}(A) = (A-\lambda I)^{-1}.$$
(31)

THEOREM 2. (Williams and Wong). Let A be a closed linear operator satisfying conditions (30) and (31) with the same Δ and m and such that there is a positive η with $\omega_1 \geqslant \eta \omega(A)$. Let f(t) satisfy the conditions of Watson's lemma. Then the bounded linear operator

$$g(A) = \int_0^\infty e^{-At} f(t) dt$$
 (32)

has the asymptotic expansion

$$g(A) \sim \sum_{k=1}^{\infty} a_k \Gamma(k/r) A^{-k/r}$$
 as $||A^{-1}|| \to 0$. (33)

Now our condition (6) is related to the condition (30). Let A be an $n \times n$ matrix which satisfies (7) and (30). We want to show that A satisfies the condition (31), and the remaining hypothesis of Theorem 1.

Write the Jordan normal form of A as

$$J = P^{-1}AP = (\lambda_1 I + U_1) \oplus \cdots \oplus (\lambda_r I + U_r),$$

$$Re(\lambda_1) \leqslant Re(\lambda_2) \leqslant \cdots \leqslant Re(\lambda_r)$$
(34)

so that U_1 has the largest of the orders of the associated unit matrices belong to λ_1 and order $U_1 = p \leqslant n = \text{order } J$. Then

$$(R_{\lambda}(A)^{m}) = (A - \lambda I)^{-m} = P(J - \lambda I)^{-m} P^{-1},$$
 (35)

and

$$(J - \lambda I)^{-m} = [(\lambda_1 - \lambda) I + U_1)]^{-m} \oplus \cdots \oplus [(\lambda_r - \lambda) I + U_r]^{-m}.$$
 (36)

Let $\lambda < \frac{1}{2} \operatorname{Re}(\lambda_1)$ whence $\operatorname{Re}(\lambda_1 - \lambda)^{-1} \ge |\lambda_j - \lambda|^{-1}$. Let ||A|| be the row sum norm subordinate to the ℓ_1 norm in \mathcal{C}^n , see Faddeeva [2, p. 58]. We need to compute $||(J - \lambda I)^{-m}||$. It suffices to evaluate

$$||Q||, Q = \{(\lambda_1 - \lambda)I + U_1\}^{-m}.$$
 (37)

But

$$Q = \begin{bmatrix} (\lambda_{1} - \lambda)^{-m} & m(\lambda_{1} - \lambda)^{-m-1} & \cdots & (m+p-1)!(\lambda_{1} - \lambda)^{-m-p}/(m-1)! \\ 0 & (\lambda_{1} - \lambda)^{-m} & \cdots & (m+p-2)!(\lambda_{1} - \lambda)^{-m-p-1}/(m-1)! \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & (\lambda_{1} - \lambda)^{-m} \end{bmatrix},$$
(38)

and so

$$||Q|| = |\lambda_1 - \lambda|^{-m} \sum_{r=0}^{p} (m+r-1)! |\lambda_1 - \lambda|^{-r}/(m-1)!.$$
 (39)

Now choose $\omega_1 = \frac{1}{2} \operatorname{Re} \lambda_1$. Then the right hand side of (39) can be bounded so that

$$\|Q\| \leqslant M_1(\omega_1 - \lambda)^{-m} \tag{40}$$

where M_1 is a positive constant which does not depend upon m. Hence

$$||R_{\lambda}(A)^{m}|| \leq n(P) M_{1}(\omega_{1} - \lambda)^{-m} = M(\omega_{1} - \lambda)^{-m}.$$
 (41)

Then for $||A^{-1}|| \to 0$, we see that inf $\omega(A) > 0$ and the hypotheses of Theorem 1 are satisfied with $\eta = \frac{1}{2}$. We have the following result.

THEOREM 3. Let A be a matrix such that the conditions (7) and (30) are satisfied and $||A^{-1}|| \to 0$. Let f(t) satisfy the conditions of Watson's lemma, see (26)–(30). If g(A) is defined by (32), then g(A) has the asymptotic expansion given by (33).

As a corollary, Williams and Wong show that the condition (31) is always satisfied by normal operators on a Hilbert space and hence by normal matrices. In our treatment, the matrix A need not be normal.

III. THE EXPONENTIAL INTEGRAL

Consider

$$S(z) = ze^{z}E_{1}(z) = ze^{z}\int_{0}^{\infty} (z+t)^{-1} e^{-t} dt.$$
 (42)

We have the divergent but asymptotic expansion

$$S(z) \sim \sum_{k=0}^{\infty} (-)^k k! z^{-k},$$

$$z \mid \to \infty \qquad |\arg z| < 3\pi/2.$$
(43)

Let

$$S_n(z) = \sum_{k=0}^{n-1} (-1)^k k! z^{-k}.$$
 (44)

It is well known that if z is positive, then for any m a positive integer or zero,

$$S_{2m+2}(z) < S(z) < S_{2m+1}(z).$$
 (45)

Clearly if A is a matrix satisfying the conditions of Theorem 3, then the asymptotic expansion of S(A) is given by (43) and this series is divergent. Thus use of (43) with z a scalar or z replaced by A is limited. Now in the scalar case, there are sequences of rational approximations and Chebyshev expansions which are based on (44) which converge. This suggests that such sequences be used in the matrix case as well. The following result in matrix theory is well known, see Dunford and Schwartz [3], Gantmacher [4] or Lancaster [5]. Let $f_m(z) \to f(z)$ uniformly on a domain D. If A is an $n \times n$ matrix for which $\sigma(A) \subseteq D$, then f(A) and $f_m(A)$ are defined and $R_m(A) = f(A) - f_m(A) \to 0$ uniformly. Hence each component of the error matrix must $\to 0$, and so any matrix norm of the error must also $\to 0$.

We shall be concerned with two types of norms and it is now convenient to define them. Let $B = (b_{ij})$, i, j = 1, 2, ..., n. Then

$$||B||_1 = \max_i \sum_{i=1}^n |b_{ij}|,$$
 (46)

$$||B||_2 = \max ||Bx||, \quad ||x|| = 1 \text{ in the Euclidean sense.}$$
 (47)

If B^* is the complex conjugate transpose of B, then

$$||B||_2^2 = \text{largest eigenvalue of } BB^*, \tag{48}$$

and if B is Hermitian,

$$||B||_2 = \text{largest eigenvalue of } B.$$
 (49)

Another important consideration for $||B||_2$ is that if B is Hermitian and positive definite, then any inequality satisfied by f(z) must also be satisfied by f(A), see [6. p. 271]. In particular, if A is Hermitan and positive definite, then from (45)

$$||S_{2m+2}(A)||_2 < ||S(A)||_2 < ||S_{2m+1}(A)||_2.$$
 (50)

To clarify some of the numerics in the next section, it is helpful to present some data for certain Padé approximations for S(z). For material on Padé

approximation and in particular for the first subdiagonal and main diagonal Padé approximations for S(z), see Luke [7, 8]. Let us write

$$S(z) = C_{n,a}(z) + R_{n,a}(z),$$
 (51)

$$C_{n,a}(z) = z^n A_{n-a}(z)/z^n B_n(z)$$
 (52)

where $A_{n-a}(z)$ and $B_n(z)$ are polynomials in z^{-1} of degree n-a and n respectively with a=0 (main diagonal Padé) or a=1 (first subdiagonal Padé). Also $R_{n,a}(z)$ is the remainder. Thus

$$C_{0,0}(z) = 1,$$
 $C_{1,0}(z) = \frac{z+1}{z+2},$ $C_{2,0}(z) = \frac{z^2+5z+2}{z^2+6z+6},$ $C_{0,1}(z) = 0,$ $C_{1,1}(z) = \frac{z}{z+1},$ $C_{2,1}(z) = \frac{z^2+3z}{z^2+4z+2},$ (53)

and further entries are readily generated by the use of a recurrence formula, see the cited references. The Padé approximations have the property that

$$B_n(z) S(z) - A_{n-a}(z) = O(z^{-2n+a-1}).$$
 (54)

Also

$$\lim_{n\to\infty} R_{n,a}(z) = 0, \quad z \text{ fixed}, \quad |\arg z| < \pi.$$
 (55)

Further, we have the important inequality,

$$C_{n,1}(z) < S(z) < C_{n,0}(z), \qquad z > 0,$$
 (56)

with equality as $z \to \infty$ provided n > 0.

Another important class of representations treated in Luke [7, 8] are expansions in series of shifted Chebyshev polynomials of the first kind $T^*(y)$. In particular, we have

$$S(x) = S_N^*(x) + R_N^*(x), \qquad S_N^*(x) = \sum_{k=0}^{N-1} c_k T_k^*(5/x), \quad x \geqslant 5.$$
 (57)

The series is convergent, that is

$$\lim_{N \to \infty} R_N^*(x) = 0. {(58)}$$

and since $|T_n^*(y)| \le 1$ for $0 \le y \le 1$, we have

$$|R_N^*(x)| \leq C_N = \sum_{k=N}^{\infty} |c_k|.$$
 (59)

The c_k 's are given to 20 decimals in the sited sources. Like coefficients for many other special functions are also recorded. If the coefficients c_k decrease with sufficient rapidity as is the case for the exponential integral, only one or two terms of the bounding series is enough to furnish a realistic appraisal of the error. Clearly (57) holds with x replaced by A provided the eigenvalues of $B = 5A^{-1}$, call them μ are such that $0 < \mu \le 1$. Also the backward recurrence technique for the evaluation of $S_N(x)$ readily carries over to the matrix case. In place of (59), we can make use of the norm noted in (47–49). So

$$||R_N^*(A)||_2 \leqslant C_N. \tag{60}$$

IV. NUMERICAL EXAMPLES

Example 1. Let

$$A = \begin{pmatrix} 14 & 10 \\ -5 & -1 \end{pmatrix}$$
 with eigenvalues 9 and 4.

Now the values of $ze^z E_1(z)$ for z=9 and 4 are 0.90775 7602 and 0.82538 2600, respectively. Then by use of the Lagrange-Sylvester representation, we get

$$S(A) = \begin{pmatrix} 0.99013 & 2604 & 0.16475 & 0004 \\ -0.08237 & 5002 & 0.74300 & 7598 \end{pmatrix}.$$

Values of $S_n(A)$ can be computed in a straight forward manner. This has been done for n = 1, 2, 3, 4. These data are omitted, but in the table below we give $||S_n(A)||_r$, r = 1, 2 for n as above.

n	$ S_n(A) _1$	$ S_n(A) _2$	
 1	1.0	1.0	
2	1.30556	1.06512	
3	1.02932	0.95716	
4	1.27765	1.05982	

The true values are $||S(A)||_1 = 1.15488$ and $||S(A)||_2 = 1.00558$. Note that the inequality (45) does not hold for the norms. According to the numerics, the inequality would be satisfied if the roles of $S_{2m+2}(z)$ and $S_{2m+1}(z)$ were interchanged. We know of no theorems in this connection save that we cannot guarantee an inequality patterned after (45) because A is not symmetric.

In the following table, we present data for the Padé approximations for S(A) described in the previous section.

n	$\ C_{n,1}(A)\ _1$	$\ C_{n,0}(A)\ _1$	$\ C_{n,1}(A)\ _2$	$\ C_{n,0}(A)\ _2$	
0	0	1.0	0	1.0	
1	1.2	1.13636	0.98033	0.99838	
2	1.15966	1.15294	1.00755	1.00477	
4		1.15484	_	1.00556	
∞	1.15488	1.15488	1.00558	1.00558	

In this table the dash means that this entry was not computed. Note that the matrix norm analog of (56) does not hold. To illustrate the approximation process, we record

$$C_{4,0}(A) = \begin{pmatrix} 0.99011 & 87 & 0.16472 & 19 \\ -0.08236 & 09 & 0.74303 & 59 \end{pmatrix}.$$

Example 2. Let

$$A = \begin{pmatrix} 8 & 2 \\ 2 & 5 \end{pmatrix}$$
 with eigenvalues 9 and 4.

The calculations are the same as those for Example 1. We therefore state the results and keep the discussion to a minimum.

$$S(A) = \begin{pmatrix} 0.89128 & 2602 & 0.03245 & 0001 \\ 0.03295 & 0001 & 0.84185 & 7600 \end{pmatrix}$$

$$\frac{n \quad ||S_n(A)||_1 \quad ||S_n(A)||_2}{1 \quad 1.0 \quad 1.0}$$

$$2 \quad 0.91667 \quad 0.88889$$

$$3 \quad 0.92130 \quad 0.91358$$

$$4 \quad 0.93017 \quad 0.90535$$

The true values are $||S(A)||_1 = 0.92423$ and $||S(A)||_2 = 0.90776$.

n	$\ C_{n,1}(A)\ _1$	$ C_{n,0}(A) _1$	$ C_{n,1}(A) _2$	$\ C_{n,0}(A)\ _2$
0	0	1.0	0	1.0
1	0.92000	0.92424	0.90000	0.90909
2	0.92437	0.92414	0.90756	0.90780
4		0.92423	_	0.90776
∞	0.92423	0.92423	0.90776	0.90776

Note that A is symmetric and positive definite so that the matrix norm analogs of (45) and (56) with norm defined by (49) hold. It is instructive to record

$$C_{4,0}(A) = \begin{pmatrix} 0.8912856 & 0.0329444 \\ 0.0329444 & 0.8418690 \end{pmatrix}.$$

EXAMPLE 3.

$$A = \begin{pmatrix} 9 & 2 \\ 2 & 6 \end{pmatrix}$$
 with eigenvalues 10 and 5.

For x = 5 and 10, we have S(x) = 0.85211 0880 and 0.91563 3339 respectively. So

$$S(A) = \begin{pmatrix} 0.902928847 & 0.025408984 \\ 0.025408984 & 0.864815372 \end{pmatrix}.$$

For application of (57) note that the eigenvalues of $B = 5A^{-1}$ are 1 and $\frac{1}{2}$. With N = 6 and the values of the c_k 's given in [4, 5], we find

$$S_6^*(A) = \begin{pmatrix} 0.9029296 & 0.0254098 \\ 0.0254098 & 0.8648147 \end{pmatrix}.$$

Also $C_6 = 0.150 \cdot 10^{-5}$.

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