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Composite Exponential Approximations

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Abstract. The Composite Exponential Approximations (CEA) arise in a natural way when one investigates the stability and order properties of a combination of several methods for the numerical solution of ordinary differential equations, sequentially implemented with different step-lengths. Some general results on the order, acceptability and exponential fitting properties of CEA are derived. The composite Padé approximations and N-approximations are explored in detail.

1. Introduction. This paper gives a theory which is relevant to the use of variable step-length to increase the order of solution of stiff ordinary differential systems. In a nutshell, we explore the effect of combining two (or more) different numerical methods with different step-lengths so that the numerical order is increased, while other desirable properties of the solution (stability, exponential fitting, etc.) are retained.

In its spirit this work follows two trails: first, the cyclic linear multistep methods [2], [20]. These methods consist of sequential application of several (possibly zero-unstable) linear multistep schemes, each with a constant step-length, so that the outcome, as a whole, is zero-stable and of high order. Second, the use of an a priori determined sequence of step-lengths (with a single method) in order to try and minimize the global error [6], [7], [13], [15].

In the sequel, instead of considering the methods themselves, we examine exponential approximations, where an exponential approximation (stability function) which corresponds to a given method is the solution by the method of the linear scalar test equation $y' = ay$, $y(0) = 1$, with unit step-length. The theory of these composite exponential approximations is much more general and uniform than separate examination of each family of numerical methods, and it answers directly the questions of A-stability and exponential fitting. As far as order is concerned, the way back from exponential approximations to methods is less straightforward. It will be described in detail in a forthcoming paper, which gives particular attention to Obrechkoff, Adams-Nørsett, implicit and semiexplicit Runge-Kutta methods. By using the given theory of composite exponential approximations that paper will develop numerical methods which have order, A-stability and exponential fitting properties superior to the existing schemes. For example, it will be shown that a two-stage A-stable semiexplicit Runge-Kutta process of order four and an exponentially fitted ν-stage A-stable implicit Runge-Kutta scheme of order 2ν can be obtained.

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In Section 2 we examine the basic model of composite exponential approximations, give some existence results and explore the connection between them and the concept of dominant pairs [8].

Section 3 is devoted to Padé approximations and to their generalizations, while Section 4 investigates the Nørsett approximations.

2. Composite Exponential Approximations. Let $R_1, \ldots, R_N$ be rational approximations to $\exp(x)$ such that $R_i(x) - \exp(x) = O(|x|^{p+1})$, $i = 1, \ldots, N$, and let $d_1 \ldots, d_N$ be arbitrary positive numbers such that $\sum_{i=1}^N d_i = 1$. Then the *Composite Exponential Approximation* (*CEA*) is defined as

$$R(x; d_1, \ldots, d_N) = R_1(d_1 x) R_2(d_2 x) \cdots R_N(d_N x). \tag{2.1}$$

It follows that $R(x; d_1, \ldots, d_N) - \exp(x) = O(|x|^{p+1})$.

We restrict our attention to positive d_i's, because they correspond to forward integration of a system of ordinary differential equations.

In the sequel we will be interested in the following problems:

(i) order: whether $d_1, \ldots, d_N$ exist so that $R(x; d_1, \ldots, d_N) - \exp(x) = O(|x|^{p+s+1})$ for $s \geq 1$, in particular for $s = N$.

(ii) exponential fitting: whether $d_1, \ldots, d_N$ exist so that the equation $R(\lambda; d_1, \ldots, d_N) = \exp(\lambda)$ holds for certain negative real values of λ.

(iii) A-acceptability: whether the approximation $R(x; d_1, \ldots, d_N)$ is A-acceptable, where we remind the reader that the exponential approximation R is A-acceptable if $|R(z)| \leq 1$ for every complex number z such that $\operatorname{Re} z \leq 0$.

In some cases, when it makes sense from the numerical point of view, we consider the less stringent A_0-acceptability criterion, which is that $|R(x)| \leq 1$ for all nonpositive real values of x.

The following sufficient condition for A-acceptability is elementary.

LEMMA 1. *If R_i, $i = 1, \ldots, N$, are A-acceptable (A_0-acceptable), then R is A-acceptable (A_0-acceptable).*

The connection between the d_k's and the order of the CEA is central to the given theory. Let

$$R_k(x) - \exp(x) = \sum_{q=p+1}^{\infty} \alpha_{k,q} x^q, \qquad 1 \leq k \leq N,$$

and

$$R(x; d_1, \ldots, d_N) - \exp(x) = \sum_{q=p+1}^{\infty} A_q(d_1, \ldots, d_N) x^q.$$

THEOREM 2. *Let $R_1, \ldots, R_N$ be rational exponential approximations of order p and let s be an integer between 1 and $p + 1$. Then the CEA $R(x; d_1, \ldots, d_N) = \prod_{k=1}^N R_k(d_k x)$ is of order $p + s$ at least if and only if*

$$\sum_{k=1}^{N} \left(\sum_{i=0}^{r-p-1} \frac{(-1)^i}{i!} \alpha_{k,r-i} \right) d_k^r = 0, \qquad p + 1 \leq r \leq p + s.$$

Proof. We set

$$\tilde{d}_k = d_k / \sum_{j=1}^{N-1} d_j, \qquad 1 < k \leq N-1, \text{ and } \tilde{R}(x; \tilde{d}_1, \ldots, \tilde{d}_{N-1}) = \prod_{k=1}^{N-1} R_k(\tilde{d}_k x)$$

and assume that

$$\tilde{R}(x; \tilde{d}_1, \ldots, \tilde{d}_{N-1}) = \sum_{q=p+1}^{\infty} \tilde{A}_q(\tilde{d}_1, \ldots, \tilde{d}_{N-1}) x^q.$$

We are interested in deriving an explicit form of A_q as a function of the $\alpha_{k,q}$'s and the d_k's. First we find a relation between A_q and $\tilde{A}_q$:

$$\sum_{q=p+1}^{\infty} A_q(d_1, \ldots, d_N) x^q$$
$$= \prod_{k=1}^{N} R_k(d_k x) - e^x = \prod_{k=1}^{N-1} R_k\left(\tilde{d}_k \sum_{j=1}^{N-1} d_j x\right) R_N(d_N x) - e^x$$
$$= \left\{ \exp\left(\sum_{j=1}^{N-1} d_j x\right) + \sum_{q=p+1}^{\infty} \tilde{A}_q(\tilde{d}_1, \ldots, \tilde{d}_{N-1}) \left(\sum_{j=1}^{N-1} d_j\right)^q x^q \right\}$$
$$\times \left\{ e^{d_N x} + \sum_{q=p+1}^{\infty} \alpha_{N,q} d_N^q x^q \right\} - e^x.$$

Therefore, for every $p + 1 \leq q \leq 2p + 1$, $\sum_{j=1}^{N} d_j = 1$ implies

$$A_q(d_1, \ldots, d_N) = \sum_{i=0}^{q-p-1} \frac{1}{i!} \tilde{A}_{q-i}(\tilde{d}_1, \ldots, \tilde{d}_{N-1}) \left(\sum_{j=1}^{N-1} d_j\right)^{q-i} d_N^i$$
$$+ \sum_{i=0}^{q-p-1} \frac{1}{i!} \alpha_{N,q-i} d_N^{q-i} \left(\sum_{j=1}^{N-1} d_j\right)^i$$
$$= \sum_{i=1}^{q-p-1} \frac{1}{i!} \left\{ d_N^{q-i}(1 - d_N)^i \alpha_{N,q-i} \right.$$
$$\left. + (1 - d_N)^{q-i} d_N^i \tilde{A}_{q-i}(\tilde{d}_1, \ldots, \tilde{d}_{N-1}) \right\}.$$

But firstly, the order of multiplication in the definition of R does not matter, and so A_q is symmetric in $(\{\alpha_{k,r}\}_{r=p+1}^{\infty}, d_k)$, $1 \leq k \leq N$. Secondly, the $\alpha_{k,q}$'s are independent of the d_k's. Hence

$$A_q(d_1, \ldots, d_N) = \sum_{i=0}^{q-p-1} \frac{1}{i!} \sum_{k=1}^{N} \alpha_{k,q-i} d_k^{q-i} (1 - d_k)^i$$

for every $p + 1 \leq q \leq 2p + 1$.

Let

$$B_r(d_1, \ldots, d_N) = \sum_{j=0}^{N} \sum_{i=0}^{r-p-1} \frac{(-1)^i}{i!} \alpha_{j,r-1} d_j \quad \text{for } p + 1 < r \leq 2p + 1.$$

By changing the order of summation and shift of indices, for every $p + 1 \leqslant q \leqslant 2p + 1$,

$$\begin{aligned} A_q(d_1, \ldots, d_N) &= \sum_{i=0}^{q-p-1} \frac{1}{i!} \sum_{k=1}^{N} \alpha_{k,q-i} d_k^{q-i} \sum_{r=0}^{i} \binom{i}{r} (-1)^r d_k \\ &= \sum_{r=p+1}^{q} (-1)^r \sum_{i=q-r}^{q-p-1} \frac{(-1)^{q-i}}{i!} \binom{i}{r-q+i} \sum_{k=1}^{N} \alpha_{k,q-i} d_k^r \\ &= \sum_{r=p+1}^{q} \frac{(-1)^r}{(q-r)!} \sum_{i=0}^{r-p-1} \frac{(-1)^{i+r}}{i!} \sum_{k=1}^{N} \alpha_{k,r-i} d_k^r \\ &= \sum_{r=p+1}^{q} \frac{1}{(q-r)!} B_r(d_1, \ldots, d_N). \end{aligned}$$

Let us suppose that $R(x; d_1, \ldots, d_N) - \exp(x) = O(x^{p+s+1})$, where $1 \leqslant s \leqslant p + 1$. Then $A_q(d_1, \ldots, d_N) = 0$ for every q between $p + 1$ and $p + s$. But

$$A_q(d_1, \ldots, d_N) = \sum_{r=p+1}^{q} \frac{1}{(q-r)!} B_r(d_1, \ldots, d_N), \qquad p + 1 \leqslant q \leqslant p + s,$$

is a triangular nonsingular linear algebraic system. Hence $B_r(d_1, \ldots, d_N) = 0$, $p + 1 \leqslant r \leqslant p + s$, which is the desired result. □

We use the notation $a_k = \alpha_{k,p+1}$, $b_k = \alpha_{k,p+2}$, $1 \leqslant k \leqslant N$. Hence $R_k(x) - \exp(x) = a_k x^{p+1} + b_k x^{p+2} + O(|x|^{p+3})$. By Theorem 2 the necessary and sufficient condition for a CEA of order $p + 1$ is

$$\sum_{k=1}^{N} a_k d_k^{p+1} = 0, \tag{2.2}$$

while the attainment of order $p + 2$ is equivalent to (2.2) together with

$$\sum_{k=1}^{N} (b_k - a_k) d_k^{p+2} = 0. \tag{2.3}$$

If $N = 2$, the condition (2.2) immediately yields the following result.

THEOREM 3. *If $R_k(x) - \exp(x) = a_k x^{p+1} + O(x^{p+2})$, $a_k \neq 0$, $k = 1, 2$, then*

(a) *If $a_1 a_2 > 0$, then no positive d_k's exist so that R is of order $p + 1$.*

(b) *If $a_1 a_2 < 0$, then there is a unique positive pair (d_1, d_2) both in the interval* '0, 1) *and given by*

$$d_1 = (-a_2/a_1)^{1/(p+1)} / \left(1 + (-a_2/a_1)^{1/(p+1)}\right),$$
$$d_2 = 1 / \left(1 + (-a_2/a_1)^{1/(p+1)}\right),$$

uch that R is of order $p + 1$.

Proof. By an examination of (2.2) for $N = 2$, namely

$$a_1 d_1^{p+1} + a_2 d_2^{p+1} = 0, \qquad d_1 + d_2 = 1. \quad □$$

No transparent existence and uniqueness result with the same scope as Theorem has been found for $N = 3$, but the following statement is useful.

THEOREM 4. *Let* $R_k(x) - \exp(x) = a_k x^{p+1} + b_k x^{p+2} + O(|x|^{p+3})$, $a_k \neq 0$, $k = 1, 2, 3$, *and let the products* $a_1 a_2$ *and* $a_2 a_3$ *be negative. If either*

$$b_2 + \eta^{p+2} b_1 > (1 - \eta) a_2, \qquad b_3 + \sigma^{p+2} b_2 < (1 - \sigma) q_3, \tag{2.4}$$

where $\eta = (-a_2/a_1)^{1/(p+1)}$, $\sigma = (-a_3/a_2)^{1/(p+1)}$ *or these two inequalities are reversed, then* d_1, d_2, d_3 *in* (0, 1) *exist,* $d_1 + d_2 + d_3 = 1$, *such that* R *is of order* $p + 2$.

Proof. We set for θ in [0, 1]

$$\begin{aligned} d^*(\theta) &= \left\{ -\left(a_1 \theta^{p+1} + a_3 (1 - \theta)^{p+1}\right)/a_2 \right\}^{1/(p+1)}, \\ d_1^*(\theta) &= \theta / (1 + d^*(\theta)), \\ d_2^*(\theta) &= d^*(\theta) / (1 + d^*(\theta)), \\ d_3^*(\theta) &= (1 - \theta) / (1 + d^*(\theta)), \end{aligned}$$

and

$$R^*(x; \theta) = R_1(d_1^*(\theta)) R_2(d_2^*(\theta)) R_3(d_3^*(\theta)).$$

It is easily seen that $\Sigma_{k=1}^3 a_k d_k^{*p+1}(\theta) = 0$ for every $\theta \in [0, 1]$. Therefore, by (2.2), R^* is of order $p + 1$ for every θ between 0 and 1.

Let $\xi(\theta) = A_{p+2}(d_1^*(\theta), d_2^*(\theta), d_3^*(\theta))$. By Theorem 2

$$\begin{aligned} \xi(\theta) = B_{p+2}(d_1^*(\theta), d_2^*(\theta), d_3(\theta)) &= \sum_{k=1}^{3} (b_k - \xi_k)[d_k^*(\theta)]^{p+2} \\ &= \frac{\left\{(b_1 - a_1)\theta^{p+2} + (b_2 - a_2)[d^*(\theta)]^{p+2} + (b_3 - a_3)(1 - \theta)^{p+2}\right\}}{(1 + d^*(\theta))^{p+2}}. \end{aligned}$$

But $d^*(0) = \sigma$, $d^*(1) = \eta$, and so

$$\begin{aligned} \xi(0) &= \left\{ b_2 \sigma^{p+2} + b_3 - a_3(1 - \sigma) \right\} / (1 + \sigma)^{p+2}, \\ \xi(1) &= \left\{ b_1 + b_2 \eta^{p+2} - a_1(1 - \eta) \right\} / (1 + \eta)^{p+2}. \end{aligned}$$

Therefore $\xi(0)\xi(1) < 0$, because of (2.4) and because σ and η are positive. Hence, by the continuity of ξ, there is θ_0 in (0, 1) such that $\xi(\theta_0) = 0$ and $R^*(x, \theta_0)$ is the desired CEA of order $p + 2$. □

Observe that conditions of the form $a_i a_j < 0$ appear in both Theorems 3 and 4. Many useful pairs of exponential approximations satisfy them.

Following [8] we call $\{R_1, R_2\}$ a *dominant pair* if for every $x \leqslant 0$

$$\min\{R_1(x), R_2(x)\} \leqslant e^x \leqslant \max\{R_1(x), R_2(x)\}. \tag{2.5}$$

If $\{R_1, R_2\}$ is dominant, then $a_1 a_2 < 0$. Hence we can use in the sequel the results of [8] and [10] to determine some exponential approximations that satisfy the conditions of Theorems 3 and 4.

In exponential fitting [14] the concept of dominant pairs is useful because of the following theorem.

THEOREM 5. *Let* $\{R_1, R_2\}$ *be a dominant pair. Then for every* $x_0 \leqslant 0$, *a* $d = d(x_0)$ *in* (0, 1) *exists such that* $R(x_0; d, 1 - d) = \exp(x_0)$.

Proof. (2.5) implies that $\exp(x_0)$ is in the interval whose endpoints are $R(x_0; 0, 1)$ and $R(x_0; 1, 0)$. The required result follows from the fact that $R(x_0; d, 1-d)$ is a continuous function of d. □

Two possible algorithms for computing the number $d(x_0)$ of Theorem 5 are:

(a) To approximate $d(x_0)$ by a rational function initially and then to iterate by the Newton-Raphson method.

(b) To use bisection, based on the fact that $d(x_0)$ is in the interval [0, 1].

3. Padé-Type Approximations. The Padé approximations to $\exp(x)$ have the form

$$R_{n,m}(x) = P_{n,m}(x)/Q_{n,m}(x),$$

$$P_{n,m}(x) = \sum_{k=0}^{m} \frac{(n+m-k)!m!}{(n+m)!k!(m-k)!} x^k, \qquad Q_{n,m}(x) = P_{m,n}(-x),$$

and they satisfy $R_{n,m}(x) - \exp(x) = O(x^{n+m+1})$. According to [3], [21], and [22] the only A-acceptable Padé approximations are $R_{n,n}$, $R_{n+1,n}$, $R_{n+2,n}$, $n = 0, 1, \ldots,$ while all the approximations $R_{n,m}$, $n \geqslant m$, are A_0-acceptable. According to [8] the pair $\{R_{n_1,m_1}, R_{n_2,m_2}\}$ is dominant if and only if $m_1 + m_2$ is odd.

LEMMA 6. *The coefficients of the equation*

$$R_{n,m}(x) - \exp(x) = a_{n,m}x^{n+m+1} + b_{n,m}x^{n+m+2} + O(x^{n+m+3})$$

have the values

$$a_{n,m} = (-1)^{n-1} \frac{m!n!}{(n+m)!(n+m+1)!},$$

$$b_{n,m} = (-1)^{n-1} \frac{m!n!(2n^2+2nm+3n+m)}{(n+m)!(n+m+2)!(n+m)}.$$

Proof. From [9] we obtain

$$P_{n,m}(x) - e^x Q_{n,m}(x) = (-1)^{n-1} \sum_{k=n+m+1}^{\infty} \frac{m!(k-m-1)!}{(n+m)!k!(k-n-m-1)!} x^k.$$

The result follows from this equation and from

$$[Q_{n,m}(x)]^{-1} = 1 + \frac{n}{n+m}x + O(x^2). \quad \square$$

Particular cases of CEA composed of two Padé approximations can be treated using Theorem 3 and Lemma 6. For instance the following two pairs of Padé approximations are of interest:

(a) $R_1 = R_{n,n}$, $R_2 = R_{n+1,n-1}$.

In this case $d_1 = d^*/(1+d^*)$, $d_2 = 1/(1+d^*)$, where $d^* = (1+1/n)^{1/(2n+1)}$. The CEA is of order $2n+1$ and it is L-acceptable (i.e., A-acceptable and tending to zero as Re $x \to -\infty$).

(b) $R_1 = R_{n,n-1}$, $R_2 = R_{n-1,n}$.

In this case $d_1 = d_2 = \frac{1}{2}$. The CEA is of order $2n$. Observe that $R_{n-1,n}$ cannot be even A_0-acceptable, but Theorem 9, which is stated and proved later, implies that the CEA is A-acceptable.

(c) Theorem 4 gives a sufficient condition for the existence of a CEA of order $p + 2$ composed out of three Padé approximations. If $R_1 = R_{n-1,m+1}$, $R_2 = R_{n,m}$, $R_3 = R_{n+1,m-1}$, then a_1a_2, $a_2a_3 < 0$ and after some algebra the conditions of the conclusion reduce to $A_1(n, m)A_2(n, m) > 0$, where

$$(3.1)\qquad \begin{aligned} A_1(n, m) &= 2\left(\frac{n}{m+1}\right)^{1/(n+m+1)} - (n - m)\left(\left(\frac{n}{m+1}\right)^{1/(n+m+1)} - 1\right), \\ A_2(n, m) &= 2 - (n - m)\left(\left(\frac{n+1}{m}\right)^{1/(n+m+1)} - 1\right). \end{aligned}$$

It can be shown that $A_1(n, m)$ and $A_2(n, m)$ are positive for every natural n and m. Therefore a CEA of this type exists for every choice of n and m.

In particular, according to Lemma 6, $a_{nn} = b_{nn}$. Hence, if $R_{n,n}$ appears among the R_k's, it is straightforward to calculate the d_k's that satisfy formulae (2.2) and (2.3). For instance, when $m = n$, we have the following case:

(c′) $R_1 = R_{n-1,n+1}$, $R_2 = R_{n,n}$, $R_3 = R_{n+1,n-1}$.

The conditions (3.1) are satisfied. Furthermore, from (2.4), (2.5) we derive

$$d_1 = d_3 = d^*/ (1 + 2d^*), \qquad d_2 = 1/ (1 + 2d^*),$$

where $d^* = (n/(2(n + 1)))^{1/(2n+1)}$.

Hence $R(x; d_1, d_2, d_3)$ is of order $2n + 2$.

LEMMA 7. *The CEA R, as defined above, is A-acceptable.*

Proof. Because of the maximum modulus theorem, it is sufficient to prove that R is analytic in the complex left half-plane and that $|R(it; d_1, d_2, d_3)|^2 \leqslant 1$ for every real t. Because the d_k's are positive the analyticity of the R_k's in the left half-plane would imply the analyticity of R. R_2 and R_3 are analytic there by [21] and [3], respectively. The required analyticity of $R_1 = R_{n-1,n+1}$ occurs if the denominator $Q_{n-1,n+1}$ has no zeros in the left half-plane. But $Q_{n-1,n+1}(z) = P_{n+1,n-1}(-z)$, and so it is sufficient to show that all the zeros of $P_{n+1,n-1}$ are in the left half-plane.

We proceed as in [3].

According to Wimp [23] all the zeros of the Bessel polynomial

$$P_n^{(a)}(z) = \sum_{k=0}^{n} \binom{n}{k}(n + a)_k z^{n-k}, \qquad a \geqslant 0, n \geqslant 1,$$

where $(n + a)_0 = 1$, $(n + a)_k = (n + a)(n + a + 1) \cdots (n + a + k - 1)$ for $k \geqslant 1$, lie in the left half-plane. Because

$$P_{n+1,n-1}(z) = \sum_{k=0}^{n-1} \frac{(2n - k)!\,(n - 1)!}{(2n)!k!\,(n - 1 - k)!} z^k = \frac{(n + 1)!}{(2n)!} P_{n-1}^{(3)}(z),$$

it follows that R_1, and consequently R, are analytic in the left half-plane.

Let $R = P/Q$. When $z = it$ the definitions of $P_{n,m}$ and $Q_{n,m}$ and the identity $d_1 = d_3$ imply

$$\begin{aligned} &|Q(it; d_1, d_2, d_3)|^2 - |P(it; d_1, d_2, d_3)|^2 \\ &\quad = |Q_{n-1,n+1}(\mathrm{i}d_1 t)Q_{n,n}(\mathrm{i}d_2 t)Q_{n+1,n-1}(\mathrm{i}d_3 t)|^2 \\ &\qquad - |P_{n-1,n+1}(\mathrm{i}d_1 t)P_{n,n}(\mathrm{i}d_2 t)P_{n+1,n-1}(\mathrm{i}d_3 t)|^2 \equiv 0. \end{aligned}$$

Hence the modulus of the rational function $R(z) = P(z; d_1, d_2, d_3)/Q(z; d_1, d_2, d_3)$ is one when z is on the imaginary axis, which completes the proof of the lemma. □

(d) $R_1 = R_{n,n}, R_2 = R_{n+1,n-1}, R_3 = R_{n+2,n-2}, n \geq 2$.

Once again (3.1) shows the existence of a CEA of order $2n + 2$, while by (2.2), (2.3) we find the coefficients

$$d_1 = d_1^*/(1 + d_1^* + d_2^*), \quad d_2 = d_2^*/(1 + d_1^* + d_2^*), \quad d_3 = 1/(1 + d_1^* + d_2^*),$$

where

$$d_1^* = \left(\frac{(n+1)(n+2)}{n(n-1)}\left(2\left(\frac{n-1}{2(n+2)}\right)^{1/(2n+2)} - 1\right)\right)^{1/(2n+1)},$$

$$d_2^* = (2(n+2)/(n-1))^{1/(2n+2)}.$$

This CEA is A_0-acceptable.

Let us now turn our attention to exponential fitting. By Theorem 5 and [8], if $R_1 = R_{n,m}$ and $R_2 = R_{n+1,m-1}$, there is a CEA of order $n + m$ that can be exponentially fitted to an arbitrary negative argument (because $\{R_{n,m}, R_{n+1,m-1}\}$ is a dominant pair). If $n = m$ then the CEA is A-acceptable.

Hence we can obtain exponentially fitted L-acceptable CEA of order $2n$ with denominators of degree n and $n + 1$. For computational reasons we are interested in denominators of degrees as small as possible. The following example shows that if we settle for A-acceptability then, under some restrictions, we can obtain exponentially fitted CEA of order $2n$, where the denominator of each rational function is of degree n.

(e) Let

$$R_1(x; \alpha) = \frac{(1-\alpha)P_{n,n-1}(x) + \alpha P_{n,n}(x)}{(1-\alpha)Q_{n,n-1}(x) + \alpha Q_{n,n}(x)},$$

$$R_2(x; \alpha) = \frac{(1-\alpha)P_{n-1,n}(x) + \alpha P_{n,n}(x)}{(1-\alpha)Q_{n-1,n}(x) + \alpha Q_{n,n}(x)}.$$

If $\alpha \in [0, 1]$ then, by [4], R_1 is A-acceptable.

Furthermore, both R_k's are of order $2n - 1$ for any α. We will form a CEA of order $2n$ from R_1 and R_2. Its properties are given in Theorem 9, which depends on the following lemma.

LEMMA 8. *For every α in* [0, 1] *the function* $Q(x; \alpha) = (1-\alpha)Q_{n-1,n}(x) + \alpha Q_{n,n}(x)$ *has no zeros for* $\operatorname{Re} x \leq 0$.

Proof. First we use a technique from the proof of Lemma 7 to show that $Q_{n-1,n}$ has no zeros in the left half-plane. The function value $Q_{n-1,n}(z)$ is equal to $P_{n,n-1}(-z)$, and the equation

$$P_{n,n-1}(z) = \frac{n!}{(2n-1)!} P_{n-1}^{(2)}(z)$$

holds, where $P_{n-1}^{(2)}$ is a Bessel polynomial. Therefore by [23] all the zeros of $Q_{n-1,n}$ are in the right half-plane.

We continue as in [5]; by deducing a contradiction from the assumption that α^* in (0, 1) and z^*, Re $z^* \leqslant 0$, exist so that $Q(z^*; d^*) = 0$. Because $Q(z; 1) = Q_{n,n}(z) \neq 0$ and $Q(z; 0) = Q_{n-1,n}(z) \neq 0$ for every z in the left half-plane, the assumption and the root locus property [12] imply the existence of real numbers $\tilde{t}$ and $\tilde{\alpha}$, where $\tilde{\alpha}$ is in (0, 1), such that $Q(i\tilde{t}; \tilde{\alpha}) = 0$. Hence the ratio $Q_{n,n}(i\tilde{t})/Q_{n-1,n}(i\tilde{t})$ is real; in other words the equation Im $Q_{n,n}(i\tilde{t})/Q_{n-1,n}(i\tilde{t}) = 0$ holds, which is equivalent to the condition

$$Q_{n,n}(i\tilde{t})\,\overline{Q_{n-1,n}(i\tilde{t})} - Q_{n,n}(i\tilde{t})\,\overline{Q_{n-1,n}(i\tilde{t})} = 0.$$

Because $Q_{n-1,n}(-i\tilde{t})$ and $Q_{n,n}(-i\tilde{t})$ are equal to $P_{n,n-1}(i\tilde{t})$ and $P_{n,n}(i\tilde{t})$, respectively, and because the equations

$$P_{n,n-1}(x) = P_{n,n}(x) - \frac{1}{2(2n-1)}xP_{n-1,n-1}(x),$$

$$Q_{n-1,n}(x) = Q_{n,n}(x) + \frac{1}{2(2n-1)}xQ_{n-1,n-1}(x),$$

are given in [5], it follows that the identity

$$Q_{n,n}(i\tilde{t})P_{n-1,n-1}(i\tilde{t}) + P_{n,n}(i\tilde{t})Q_{n-1,n-1}(i\tilde{t}) = 0$$

is obtained, which is the same as the equation

$$\text{Re } Q_{n,n}(i\tilde{t})P_{n-1,n-1}(i\tilde{t}) = 0.$$

The polynomial Re $Q_{n,n}(i\tilde{t})P_{n-1,n-1}(i\tilde{t})$ is even and, according to [5], the even-powered terms of $Q_{n,n}(z)P_{n-1,n-1}(z)$ are

$$E_{n,n-1}(z) = \frac{2n!\,(n-1)!}{(2n-2)!\,(2n)!}\sum_{j=0}^{n-1}\frac{(2n-2j-2)!\,(2n-j-1)!}{j!\,((n-j-1)!)^2}(-z^2)^j.$$

Hence Re $Q_{n,n}(i\tilde{t})P_{n-1,n-1}(i\tilde{t}) = E_{n,n-1}(i\tilde{t}) > 0$. This contradiction completes the proof. □

THEOREM 9. *Let R_1 and R_2 be as defined above and let $R = R(x; \alpha)$ be the corresponding CEA with $d_1 = d_2 = \frac{1}{2}$. Then*

(i) *R is A-acceptable for every α in* [0, 1].

(ii) *For every α, $R(x; \alpha) - \exp(x) = O(x^{2n+1})$.*

(iii) *$x_0 < 0$ exists such that, for every $x^* \leqslant x_0$, there is an $\alpha = \alpha(x^*)$ in* [0, 1] *so that $R(x^*; \alpha) = \exp(x^*)$.*

Proof. (i) By Lemma 8 and the A-acceptability of R_1, R is analytic in the left half-plane. Furthermore, for every α and real t, $|R(it; \alpha)| \equiv 1$. The acceptability follows.

(ii) The order of R is proved by combining Theorem 3 and Lemma 6, using the identity $Q_{n,m}(0) = 1$.

(iii) By examining coefficients we find that, for $x \ll 0$, $R(x; 0) < 0 < \exp(x)$. Moreover, because $R(x; 1) = R_{n,n}^2(\frac{1}{2}x) > 0$, and because the decay of rational functions is necessarily slower than that of $\exp(x)$, we deduce $R(x; 1) > \exp(x)$ when $x \ll 0$.

Therefore $x_0 < 0$ exists such that, for every $x \leqslant x_0$,

$$R(x; 0) < \exp(x) < R(x; 1).$$

Since R is continuous in α for $\alpha \in [0, 1]$, it follows that, for every $x^* \leq x_0$, $\alpha = \alpha(x^*)$ exists such that $R(x^*, \alpha) = \exp(x^*)$, which is the required result. □

Table I gives the greatest x_0 that is allowed by Theorem 9 for $1 \leq n \leq 10$.

TABLE I. *The x_0's for $n = 1, \ldots, 10$.*

n	x_0
1	−4.7987
2	−5.5882
3	−10.0729
4	−10.9024
5	−15.3653
6	−16.2086
7	−20.6624
8	−21.5127
9	−25.9615
10	−26.8159

Remark. The principal error term (i.e., the coefficient of x^{2n+1} in the error expansion) of $R(x; \alpha)$ has the value

$$E_n(\alpha) = \frac{(-1)^{n-1}(n!)^2}{2^{2n}((2n)!)^2(2n-1)}\left(\frac{4n}{2n+1} - 2\alpha + \alpha^2\right).$$

Because $\alpha^2 - 2\alpha + 4n/(2n+1) \neq 0$ for every $n \geq 1$ and real α, the order $2n$ cannot be increased. Furthermore, $|E_n(\alpha)|$ attains its minimum value when $\alpha = 1$, which corresponds to two equal steps by the diagonal Padé approximation $R_{n,n}$. Therefore, as far as order and local error (but not exponential fitting) are concerned, one cannot do better than the diagonal Padé approximation.

Remark. Higher orders of the CEA can be attained by allowing complex d_k's, complex R_k's or R_k's such that

$$R_k(x) - \exp(x) = a_k x + O(x^2), \qquad a_k \neq 0.$$

Three examples are given:

(i) If $R_1 = R_2 = R_{1,1}$, $d_1 = \frac{1}{2} + \sqrt{3}\, i/6$, $d_2 = \frac{1}{2} - \sqrt{3}\, i/6$, then $R(x; d_1, d_2) = R_{2,2}(x)$, of order 4.

(ii) If $\alpha = 1 \pm \sqrt{(2n-1)/(2n+1)}\, i$, then the CEA of Theorem 8 is of order $2n+1$ (as can be easily verified by an examination of the principal error term).

(iii) If $s = \sqrt[3]{4(\sqrt{5}+1)} - \sqrt[3]{4(\sqrt{5}-1)}$,

$$q_1(x) = 1 - \frac{2}{4+s}x,$$

$$q_2(x) = 1 - \frac{16-2s}{16-4s+s^2-6\sqrt[3]{2}}x + \frac{4}{16-4s+s^2-6\sqrt[3]{2}}x^2,$$

$$R_1(x) = q_1(-x)/q_1(x), \quad R_2(x) = q_2(-x)/q_2(x), \text{ then}$$

$$R\left(x; \tfrac{1}{2}, \tfrac{1}{2}\right) = R_{3,3}(x), \quad \text{of order 6.}$$

However, these approximations are of little or no computational value.

4. Nørsett Approximations. Rational approximations to $\exp(x)$ with only real poles [17], [18] are of great importance in the numerical solution of large stiff systems with sparse Jacobian matrices (such systems are obtained, for example, when one solves parabolic partial differential equations by the method of lines). They are variously called multiple Padé approximations [17], N-approximations [18], and restricted Padé approximations [22]. In the following we prefer the name N-approximations.

According to Nørsett and Wolfbrandt [18], one cannot exceed order $n + 1$ if an approximation has n poles, which are all real and the degree of the numerator does not exceed n. The best such approximation, as far as local principal error is concerned, is attained by an approximation that has just one real pole, of multiplicity n. Therefore, in the sequel we restrict our attention to this type of approximation.

Let $L_n^{(d)}$ denote the generalized Laguerre polynomial [19],

$$L_n^{(d)}(x) = \frac{(1+d)_n}{n!} \sum_{k=0}^{n} (-1)^k \binom{n}{k} \frac{1}{(1+d)_k} x^k,$$

where $(1 + d)_0 = 1$, $(1 + d)_k = (1 + d)(2 + d) \cdots (k + d)$. The usual Laguerre polynomial of degree n is $L_n = L_n^{(0)}$.

Let $S_{n,k}(x) = p_{n,k}(x)/(1 - a_k x)^n$, where

$$p_{n,k}(x) = \sum_{i=0}^{n} \left(\sum_{j=0}^{i} \frac{(-1)^i}{(i-j)!} \binom{n}{j} a_k^j \right) x^i, \tag{4.1}$$

and where a_k is the reciprocal of the kth zero of $L_n^{(1)}$ (and so, according to [19], a_k is real and positive). Nørsett [17] proves that $S_{n,k}(x) - \exp(x) = c_{n,k} x^{n+2} + O(x^{n+3})$, where

$$c_{n,k} = (-1)^{n+1} \frac{1}{n+2} a_k^{n+1} L_n(1/a_k).$$

We consider in this section some CEA's that are formed from these N-approximations.

THEOREM 10. *The pair $\{S_{n,i_1}, S_{n,i_2}\}$ is dominant if and only if $i_1 + i_2$ is odd.*

Proof. According to Theorem 4.3 of [17],

$$S_{n,k}(x) - e^x = L_n(1/a_k) e^x \int_0^x (t/(t - 1/a_k))^{n+1} e^{-t}\, dt. \tag{4.2}$$

Because $a_k > 0$, the integral on the right is positive for $x < 0$. Hence it is sufficient to prove that the signs of the numbers $\{L_n(1/a_k): k = 1, 2, \ldots, n\}$ alternate. According to [19],

$$L_n(x) = L_n^{(1)}(x) - L_{n-1}^{(1)}(x).$$

Therefore the proof follows by the interlacing property of the zeros of $\{L_n^{(1)}\}_{n=0}^{\infty}$. □

(f) Let $R_1 = S_{n,i_1}$ and $R_2 = S_{n,i_2}$. Because $\operatorname{sgn} c_{n,i_1} c_{n,i_2} = (-1)^{i_1+i_2}$, it follows that, if $i_1 + i_2$ is odd, then d_1 and d_2 in $(0, 1)$ exist, such that the CEA is of order $n + 2$. In fact, according to Theorem 2,

$$d_1 = d^*/(1 + d^*); \quad d_2 = 1/(1 + d^*),$$

where

$$d^* = \left(-\left(a_{i_2}^{n+1}L_n(1/a_{i_2})\right)/\left(a_{i_1}^{n+1}L_n(1/a_{i_1})\right)\right)^{1/(n+2)}.$$

According to [22] very few N-approximations of the type $S_{n,k}$ are A-acceptable. However, owing to the special structure of the sparse Jacobian matrices, which are encountered in the numerical solution of parabolic equations by the method of lines, A_0-acceptability is frequently a suitable stability requirement.

The A_0-acceptable approximations $S_{n,k}$ are fully characterized in [17]. The following lemma gives a stability result which, although less general, is sufficient for many practical cases of CEA's of two approximations $S_{n,k}$.

LEMMA 11. *Let* $R_k = S_{n,i_k}$, $i_1 + i_2$ *odd and* $b_k = L_n(1/a_{i_k})$, $k = 1, 2$, *where* a_{i_k} *is the* i_k*th zero of* $L_n^{(1)}(1/x)$, *and let* R *be any CEA. Then*

(i) $|b_1 b_2| \leqslant 1$ *is necessary for the* A_0-*acceptability of* R.

(ii) *If* $|b_1|, |b_2| \leqslant 1$, *then* R *is* A_0-*acceptable.*

Proof. (i) According to (4.1) for $x \ll 0$

$$S_{n,i_k} \approx (-1)^n \sum_{j=0}^{n} \frac{(-1)^j}{(n-j)!}\binom{n}{j} a_{i_k}^j / a_{i_k}^n = b_k.$$

Hence for $d_1, d_2 \in (0, 1)$

$$\lim_{x\to-\infty} |R(x; d_1, d_2)| = |b_1 b_2|,$$

which shows that R is A_0-acceptable only if $|b_1 b_2| \leqslant 1$.

(ii) If $|b_1|, |b_2| \leqslant 1$, then, according to [17], both S_{n,i_1} and S_{n,i_2} are A_0-acceptable. The A_0-acceptability of R follows from Lemma 1 and Theorem 3. □

Table II gives the acceptability properties of some composite N-approximations of type (f) and, for the sake of comparison, the acceptability properties of some N-approximations $S_{n,k}$. According to [17], the A_0-acceptable N-approximations are also $A(\alpha)$-acceptable, where R is $A(\alpha)$-acceptable if $|R(z)| < 1$ for every z which belongs to the wedge-shaped domain $\{z\colon |\arg(-z)| < \alpha\}$ of the complex left half-plane [11]. It is customary to present α in degrees, rather than in radians—thus $A(90)$-acceptability corresponds to A-acceptability. As Nørsett points out in [17], for $n \leqslant 9$ the A_0-acceptable N-approximations are $A(\alpha)$-acceptable with $\alpha \geqslant 89$. As is evident from Table II, the composition preserves this property.

(g) $R_k = S_{n,i_k}$, $k = 1, 2$, $i_1 + i_2$ odd, with exponential fitting.

As a consequence of Theorem 10, for every $x_0 < 0$, d exists in (0, 1) such that $R(x_0; d, 1 - d) = \exp(x_0)$. If $x_0 < 0$ then the order is $n + 1$, while, in the limit as x_0 tends to zero, one gets the CEA of type (f).

(h) $R_k = S_{n,i_k}$, $k = 1, 2, 3$.

Table II shows the relative scarcity of acceptable N-approximations and their composite counterparts for small values of n. The least value of n for which there is an A_0-acceptable CEA of three N-approximations, whose order is $n + 3$, is $n = 6$, and the coefficients of the CEA are $i_1 = 4$, $i_2 = 5$, $i_3 = 6$, $d_1 = 0.59375$, $d_2 = 0.34375$, $d_3 = 0.06250$.

TABLE II

All the acceptable N-approximations $S_{n,i}$ and CEA $\{S_{n,i_1}, S_{n,i_2}\}$ for $2 \leqslant n \leqslant 7$

n	i_1 or i	i_2	d_1	d_2	Acceptability	Order
2	2	-	-	-	A-acc.	3
	1	2	0.341081377	0.658918623	A-acc.	4
3	3	-	-	-	A-acc.	4
	2	3	0.301016914	0.698983084	A-acc.	5
4	4	-	-	-	A-acc.	5
	3	4	0.281617072	0.718382928	$A(89)$-acc.	6
5	4	-	-	-	A-acc.	6
	5	-	-	-	$A(89)$-acc.	6
	4	5	0.270247623	0.729752377	$A(89)$-acc.	7
6	5	-	-	-	$A(89)$-acc.	7
	6	-	-	-	$A(89)$-acc.	7
	5	6	0.262827198	0.737172802	$A(89)$-acc.	8
7	6	-	-	-	$A(89)$-acc.	8
	7	-	-	-	$A(89)$-acc.	8
	5	6	0.354081725	0.645918275	A-acc.	9
	6	7	0.257628647	0.742371353	$A(89)$-acc.	9

An alternative approach to the N-approximations [17] is to let the polynomial p in the numerator be of degree $n - 1$ and to require the order of the approximation to be only n. This approach is of relevance to semiexplicit Runge-Kutta methods [16], [1]. As is conjectured by Nørsett [16] no semiexplicit Runge-Kutta method of n stages can attain order $n + 1$ for even n, $n \geqslant 4$. The exponential approximations of these methods are N-approximations. Among the N-approximations of order n the approximations with $\deg p = n - 1$ have the best asymptotic acceptability properties.

It is proven in [17] that the approximation

$$T_{n,k}(x) = p_{n,k}(x)/(1 - a_k x)^n$$

is of order n, where $P_{n,k}$ is the polynomial (4.1) and where a_k is the reciprocal of the kth zero of L_n. The choice of a_k implies $\deg p = n - 1$ and $T_{n,k}(x) - \exp(x) = c_{n,k}x^{n+1} + O(x^{n+2})$, where

$$c_{n,k} = \frac{(-1)^{n+1}}{n+1} a_k^n L_n^{(1)}(1/a_k).$$

THEOREM 12. *The pair $\{T_{n,i_1}, T_{n,i_2}\}$ is dominant if and only if $i_1 + i_2$ is odd.*

Proof. According to Theorem 4.3 in [17]

$$T_{n,k}(x) - e^x = L_n^{(1)}(1/a_k)/a_k e^x \int_0^x t^n/(t - 1/a_k)^{n+1} e^{-t}\, dt.$$

The proof proceeds along the same lines as the proof of Theorem 10. □

Hence, by Theorems 3 and 5 it is possible to form CEA of the N-approximations $T_{n,k}$ in order to exponentially fit or increase the order, while preserving the acceptability properties.

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