A-Stability and Dominating Pairs *

By Arieh Iserles

Abstract. It is considered whether linear combinations of A-acceptable exponential approximations preserve the A-stability, when the coefficients of the linear combination are selected in order to achieve exponential fitting. Various pairs of exponential approximations are discussed and the satisfactory pairs are characterized.

1. **Introduction.** The author's paper [4] presents a new family of methods for numerical solution of stiff ordinary differential systems, based on the following principle:

Let $x_{n+1}^{(l_k)}$ be the numerical solution of the system

(1.1) $$\dot{x} = f(t, x), \qquad x(t_n) = x_n \in E^N$$

at $t_{n+1} = t_n + h$, achieved by l_k equal steps of the length h/l_k, by applying the trapezoidal rule. Let Z be a family of scalar differential equations whose solutions are known in the closed form:

$$Z = \{\dot{z}_k = g_k(t, z_k), z_k(t_n) = 1, 1 \leqslant k \leqslant M\}.$$

We assume that $\{x_{n+1}^{(l_k)}\}_{k=1}^{P}$ have been computed. Thus $M = M(P)$ and a scheme

$$x_{n+1} = F(x_{n+1}^{(l_1)}, x_{n+1}^{(l_2)}, \ldots, x_{n+1}^{(l_p)}),$$

of at least the second order exist, causing the scheme to be fitted to the family Z (i.e. the scheme solves with precision the equations of Z).

The purpose of this paper is to generalize the results of [4] in a certain direction. We consider the solutions $x_{n+1}^{(1)}$ and $x_{n+1}^{(2)}$ of (1.1) obtained by any two numerical schemes at t_{n+1} and we combine them linearly, in order to gain one degree of exponential fitting:

(1.2) $$x_{n+1} = \alpha x_{n+1}^{(1)} + (1 - \alpha)x_{n+1}^{(2)}.$$

Assuming that the two considered numerical schemes are A-stable, we are confronted with a question whether the combined scheme (1.2) is A-stable. This paper is devoted to the above-mentioned question. An attempt is made to get necessary and sufficient conditions for A-stability and to analyze certain pairs of numerical schemes and their stability.

2. **The Stability and the Dominant Pairs.** If two numerical schemes for solution of stiff O.D.E.'s are given, we look upon their characteristic functions χ_1 and χ_2. The

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characteristic function $\chi(\mu)$, as defined in [5], is the solution at $h = \mu/\lambda$ of the linear scalar equation $\dot{x} = \lambda x$, $x(0) = 1$. Thus, for example, the characteristic function of the trapezoidal rule is

$$\chi(\mu) = (1 + \tfrac{1}{2}\mu)/(1 - \tfrac{1}{2}\mu),$$

the $[1, 1]$ Padé approximation to $\exp(\mu)$.

We are concerned in the sequel with numerical schemes for which the solution at $h = \mu/\lambda$ of the linear equation $\dot{x} = \lambda x$, $x(0) = x_0$, is given by $\chi(\mu)x_0$, when χ is the characteristic function. For these schemes the requirement of A-stability is, trivially, equivalent to the condition

$$|\chi(\lambda)| < 1 \quad \text{for every } \lambda, \quad \text{Re } \lambda < 0.$$

Considering the characteristic function χ of the combined scheme (1.2), we see that

(2.1) $$\chi(\mu) = \alpha\chi_1(\mu) + (1 - \alpha)\chi_2(\mu).$$

LEMMA 1. *If χ_k, $k = 1, 2$, are analytical in the left half plane and A-acceptable then the sufficient condition for A-acceptability of χ is $\alpha \in [0, 1]$. If $|\chi_k(it)| \equiv 1$ for every $t \in R$, $k = 1, 2$ also, then this is the necessary condition too.*

Proof. Clearly, this is a sufficient condition: for every z, Re $z < 0$,

$$|\chi(z)| \leq \alpha|\chi_1(z)| + (1 - \alpha)|\chi_2(z)| < \alpha + (1 - \alpha) = 1,$$

provided $0 \leq \alpha \leq 1$.

χ_k, $k = 1, 2$, are analytical, thus χ, defined by (2.1), is analytical too. Therefore, according to the maximum principle, the inequality $|\chi(it)| \leq 1$ $\forall t \in R$ is a necessary condition for A-stability. Hence,

$$|\chi(it)|^2 = \alpha^2|\chi_1(it)|^2 + (1 - \alpha)^2|\chi_2(it)|^2 + 2\alpha(1 - \alpha)\text{Re } \chi_1(it)\overline{\chi_2(it)}$$

$$= 1 + 2\alpha(\alpha - 1)(1 - \text{Re } \chi_1(it)\overline{\chi_2(it)})$$

and $|\chi(it)| \leq 1$ implies

$$\alpha(\alpha - 1)(1 - \text{Re } \chi_1(it)\overline{\chi_2(it)}) \leq 0.$$

But $|\chi_k(it)|^2 \equiv 1$ implies Re $\chi_1(it)\overline{\chi_2(it)} \leq 1$, thus

$$\alpha(\alpha - 1) \leq 0, \quad \text{ergo } \alpha \in [0, 1]. \quad \text{Q.E.D.}$$

Definition. If $\chi_1(\mu)$ and $\chi_2(\mu)$ are A-acceptable approximations to $\exp(\mu)$, we shall define the pair $\{\chi_1, \chi_2\}$ as a dominant if for every $\mu \leq 0$

(2.2) $$\min\{\chi_1(\mu), \chi_2(\mu)\} \leq e^\mu \leq \max\{\chi_1(\mu), \chi_2(\mu)\}$$

is valid.

LEMMA 2. *If $\{\chi_1, \chi_2\}$ is a dominant pair and $\chi(\mu) = \alpha\chi_1(\mu) + (1 - \alpha)\chi_2(\mu)$ is fitted to any $\lambda \leq 0$, then χ is A-acceptable.*

Proof. The inequality (2.2) implies $(\chi_1(\mu) - e^\mu)(\chi_2(\mu) - e^\mu) \leqslant 0$. But $\chi(\lambda) = \exp(\lambda)$, hence

$$\alpha = \frac{\chi_1(\lambda) - e^\lambda}{\chi_1(\lambda) - \chi_2(\lambda)} = \frac{\chi_1(\lambda) - e^\lambda}{(\chi_1(\lambda) - e^\lambda) - (\chi_2(\lambda) - e^\lambda)} = \frac{1}{1 - \dfrac{\chi_2(\lambda) - e^\lambda}{\chi_1(\lambda) - e^\lambda}}.$$

Thus, $0 \leqslant \alpha \leqslant 1$ and, according to Lemma 1, χ is A-acceptable.

This argument fails when $\chi_1(\lambda) = \chi_2(\lambda)$. But then $\chi_1(\lambda) = \chi_2(\lambda) = \exp(\lambda)$, because $\{\chi_1, \chi_2\}$ is a dominant pair, and χ is fitted to λ with every real α. We select $\alpha \in [0, 1]$ and again, χ is A-acceptable. Q.E.D.

The last lemma gives a practical tool for the stability analysis. Nevertheless, the dominancy conception is sometimes, as is shown in the sequel, too demanding. Hence, it seems nothing but natural to slacken the definition:

Definition. If $\chi_1(\mu)$ and $\chi_2(\mu)$ are A-acceptable approximations to $\exp(\mu)$, we shall define the pair $\{\chi_1, \chi_2\}$ as a λ_0-dominant pair, $\lambda_0 \leqslant 0$, if for every $\mu \leqslant \lambda_0$

$$\min\{\chi_1(\mu), \chi_2(\mu)\} \leqslant e^\mu \leqslant \max\{\chi_1(\mu), \chi_2(\mu)\}$$

is valid.

LEMMA 2*. *If $\{\chi_1, \chi_2\}$ is a λ_0-dominant pair and $\chi(\mu) = \alpha\chi_1(\mu) + (1 - \alpha)\chi_2(\mu)$ is fitted to any $\lambda \leqslant \lambda_0$, then χ is A-acceptable.*

Proof. Identical to the proof of Lemma 2.

In the following chapters three families of possible dominant or λ_0-dominant pairs are analyzed:

(a) the pairs of Padé approximations to the exponential,

$$(2.3) \qquad R_{n,m} := \frac{P_{n,m}}{Q_{n,m}}, \qquad P_{n,m} := \sum_{k=0}^{m} \frac{(m + n - k)!\,m!}{(m + n)!\,k!\,(m - k)!} z^k,$$

$$Q_{n,m} := P_{m,n}(-z);$$

(b) the pairs of the modified Padé approximants, possessing single degree of exponential fitting [2], [6],

$$R_{n,m}^{(1)}(z) := \frac{P_{n,m}(z) + \mu P_{n,m-1}(z)}{Q_{n,m}(z) + \mu Q_{n,m-1}(z)};$$

(c) the pairs of "extrapolants", i.e. results obtained with the same characteristic function but with different step lengths, being the natural generalization of the schemes considered in [4].

3. **The Padé Approximations.** The objective of this section is to analyze the dominancy property of the pairs $\{R_{n_1,m_1}, R_{n_2,m_2}\}$, when R_{n_k,m_k}, $k = 1, 2$, are Padé approximations, defined as in (2.3).

We apply certain properties of the Padé approximation, all easily derived from the explicit formulae. Most of these properties are widely known (see, for example, [1] and [3]).

Hence, we define

$$\psi_{n,m}(z) := P_{n,m}(z) - e^z Q_{n,m}(z).$$

By [3]

(3.1) $$\psi_{n,m}(z) = \frac{m}{n+m}\,\psi_{n,m-1}(z) + \frac{n}{n+m}\,\psi_{n-1,m}(z).$$

Thus, acting upon (2.3) and (3.1), we prove that

$$\frac{d}{dz}\,\psi_{n,m}(z) = \frac{m}{n+m}\,\psi_{n,m-1}(z).$$

LEMMA 3. $\psi_{n,0}(z) \geqslant 0$ *is valid for every* $z \leqslant 0$ *and* $\psi_{n,0}$ *is monotonously descending in the above-mentioned interval.*

   Proof.   By a direct differentiation:

$$\psi_{n,0}(z) = 1 - e^z \sum_{k=0}^{n} (-1)^k \frac{z^k}{k!},$$

hence

$$\psi'_{n,0}(z) = (-1)^{n+1} \frac{e^z}{n!} z^n = -\frac{e^z}{n!}(-z)^n = -\frac{e^z}{n!}|z|^n \leqslant 0$$

provided $z \leqslant 0$.

   Thus, $\psi_{n,0}$ is monotonously descending in $(-\infty, 0]$. But $\psi_{n,0}(0) = 0$; therefore,

$$\psi_{n,0}(z) \geqslant 0 \quad \forall z \leqslant 0. \quad \text{Q.E.D.}$$

THEOREM 4.   *For every* n, $m \geqslant 0$ *and* $z \leqslant 0$ *it is valid that* $(-1)^m \psi_{n,m}(z) \geqslant 0$, *and* $\psi_{n,m}$ *is monotone.*

   Proof.   By induction on m:

   We proved the validity of the theorem for $\psi_{n,0}$. Moreover, we bear in mind that

$$\psi'_{n,m}(z) = \frac{m}{n+m}\,\psi_{n,m-1}(z).$$

Thus, according to the induction assumption, $(-1)^m \psi'_{n,m}(z) \leqslant 0$ implying immediately the theorem.   Q.E.D.

   Theorem 4 can serve to derive various results on Padé approximations. For example, it is effortlessly shown that if m is even, $R_{n,m}$ has no real negative zero; and if m is odd, $R_{n,m}$ has exactly one such zero. Nevertheless, such results are outside the scope of this paper.

   Bearing in mind the result of [1], namely that $R_{n+k,n}$, $k = 0, 1, 2$, are A-acceptable, and applying Theorem 4, we readily see that

THEOREM 5.   *The pairs* $\{R_{n+k,n}, R_{m+l,m}\}$ *for* $0 \leqslant k, l \leqslant 2$, *are dominant if and only if* $n + m$ *is odd.*

   Moreover, if the Ehle conjecture [1] is valid, namely if $R_{n+k,n}$, $k = 0, 1, 2$,

are the only A-acceptable Padé approximations, then Theorem 5 characterizes completely the dominant pairs which are composed of such approximations.

4. **The Exponentially-Fitted Approximations.** Ehle in [2] defined a family of exponential approximations, possessing single degree of exponential fitting. These approximations can be defined as

$$R_{n,m}^{(1)}(z) := \frac{P_{n,m}(z) + \mu P_{n,m-1}(z)}{Q_{n,m}(z) + \mu Q_{n,m-1}(z)},$$

and if $\mu = \mu_{n,m}(\phi) := - \psi_{n,m}(\phi)/\psi_{n,m-1}(\phi)$,

$$R_{n,m}^{(1)}(\phi) = e^{\phi}.$$

Ehle in [2] and Nørsett in [6] proved that if $\phi \leqslant 0$, then $R_{n,n}^{(1)}$ and $R_{n,n-1}^{(1)}$ are A-acceptable. Moreover, by applying Theorem 4, we see that for every $\phi \leqslant 0$, $\mu(\phi) \geqslant 0$. The objective of this section is to prove that the pairs $\{R_{n+k,n}^{(1)}, R_{m+l,m}^{(1)}\}$, when $0 \leqslant k, l \leqslant 1$, are dominant if and only if $n + m$ is odd (if not stated otherwise, we assume that all the approximations are fitted at the same point).

The fundamental result, which enables the proof of the above-mentioned assertion, is that $\mu_{n,m}(\phi)$ is monotone for $\phi \leqslant 0$. This is proved by a two-stage induction:

LEMMA 6. $\mu_{1,1}(\phi)$ *is a monotonously descending function.*
Proof.

$$\mu_{1,1}(\phi) = - \frac{1 + \frac{1}{2}\phi - (1 - \frac{1}{2}\phi)e^{\phi}}{1 - (1 - \phi)e^{\phi}}$$

and by direct differentiation

$$(1 - (1 - \phi)e^{\phi})^2 \mu_{1,1}'(\phi) = - \frac{1}{2}[(1 - e^{\phi})^2 - \phi^2 e^{\phi}].$$

Let us assume $\mu_{1,1}'(\phi) = 0$. Thus $(1 - e^{\phi})^2 = \phi^2 e^{\phi}$ and provided $\phi \leqslant 0$, $1 - e^{\phi} = -\phi e^{\frac{1}{2}\phi}$. Hence, $\frac{1}{2}(e^{\frac{1}{2}\phi} - e^{-\frac{1}{2}\phi}) = \frac{1}{2}\phi$; and if $v = \frac{1}{2}\phi$,

(4.1) $v = \sinh v.$

The unique real solution of the transcendental equation (4.1) is widely known to be $v = 0$. Therefore, $\mu_{1,1}'(\phi) \neq 0$ for $\phi < 0$. But $\mu_{1,1}(0) = 0$, $\mu_{1,1}(\phi) \geqslant 0$ for $\phi < 0$ and $\mu_{1,1}(\phi)$ continuous in $(-\infty, 0]$; thus $\mu_{1,1}$ is monotonously descending. Q.E.D.

LEMMA 7. *The identity*

(4.2) $\psi_{n,0}^2(\lambda)\mu_{n,1}'(\lambda) + \dfrac{1}{n+1}\lambda^2 \psi_{n-1,0}^2(\lambda)\left(\dfrac{\mu_{n-1,1}(\lambda)}{\lambda}\right)' = 0$

is valid for every $\lambda \leqslant 0$.

Proof. We define

$$p(\lambda) := \psi_{n,0}^2(\lambda)\mu'_{n,1}(\lambda),$$

$$q(\lambda) := \lambda^2 \psi_{n-1,0}^2(\lambda)\left(\frac{\mu_{n-1,1}(\lambda)}{\lambda}\right)'.$$

Using in the sequel the identity

$$\psi'_{n,m} = \frac{m}{n+m}\psi_{n,m-1}, \quad m \geqslant 1,$$

from the last chapter, as well as the easily derived identities

$$\psi'_{n,0} = (-1)^{n+1}e^\lambda\frac{\lambda^n}{n!}, \quad \psi_{n,0} = \psi_{n-1,0} - (-1)^n\frac{\lambda^n}{n!}e^\lambda$$

and the identity

$$\psi_{n,m} = \psi_{n,m-1} + \frac{n}{(n+m)(n+m-1)}\lambda\psi_{n-1,m-1}$$

from [3], we obtain:

$$p(\lambda) = (-1)^{n+1}e^\lambda\frac{\lambda^n}{n!}\left(\psi_{n,0} + \frac{1}{n+1}\lambda\psi_{n-1,0}\right) - \frac{1}{n+1}\psi_{n,0}^2$$

and

$$q(\lambda) = \lambda\left\{(-1)^n e^\lambda\frac{\lambda^{n-1}}{(n-1)!}\left(\psi_{n-1,0} + \frac{1}{n}\lambda\psi_{n-2,0}\right) - \frac{1}{n}\psi_{n-1,0}^2\right\}$$
$$+ \psi_{n-1,0}\left(\psi_{n-1,0} + \frac{1}{n}\lambda\psi_{n-2,0}\right);$$

hence

$$p(\lambda) + \frac{1}{n+1}q(\lambda) = -\frac{1}{n(n+1)}\lambda\psi_{n-1,0}(\psi_{n-1,0} - \psi_{n-2,0})$$
$$+ (-1)^{n+1}e^\lambda\frac{\lambda^{n+1}}{(n+1)!}(\psi_{n-1,0} - \psi_{n-2,0})$$
$$+ \frac{1}{n+1}(\psi_{n-1,0} - \psi_{n,0})(\psi_{n-1,0} + \psi_{n,0})$$
$$+ (-1)^{n+1}e^\lambda\frac{\lambda^n}{(n-1)!}\left(\frac{1}{n}\psi_{n,0} - \frac{1}{n+1}\psi_{n-1,0}\right).$$

It can easily be shown that

$$\frac{1}{n}\psi_{n,0} - \frac{1}{n+1}\psi_{n-1,0} = \frac{1}{n(n+1)}\psi_{n-1,0} - \frac{(-1)^n}{n\cdot n!}\lambda^n e^\lambda$$

implying

$$p(\lambda) + \frac{1}{n+1} q(\lambda) = \frac{(-1)^{n+1}}{(n+1)!} e^{\lambda} \lambda^n \psi_{n-1,0} - e^{2\lambda} \frac{\lambda^{2n}}{(n-1)!(n+1)!}$$

$$+ \frac{(-1)^n}{(n+1)!} e^{\lambda} \lambda^n (\psi_{n-1,0} + \psi_{n,0})$$

$$+ \frac{(-1)^{n+1}}{(n+1)!} e^{\lambda} \lambda^n \psi_{n-1,0} + e^{2\lambda} \frac{\lambda^{2n}}{(n!)^2}$$

$$= \frac{1}{n!(n+1)!} \lambda^{2n} e^{2\lambda} + \frac{(-1)^n}{(n+1)!} \lambda^n e^{\lambda} (\psi_{n,0} - \psi_{n-1,0}) = 0.$$

<div align="right">Q.E.D.</div>

The apparent conclusion of Eq. (4.2) is:

LEMMA 8. *For every $n \geq 1$ and $\lambda \leq 0$ the function $\mu_{n,1}(\lambda)$ descends monotonously.*

Proof. In Lemma 6 this result was proved for $n = 1$. Assuming by induction that $\mu_{n-1,1}(\lambda)$ is descending for $\lambda < 0$ and bearing in mind that $\mu_{n-1,1}(\lambda) \geq 0$ and that $K(\lambda) = 1/\lambda$ is negative and descending in this interval, we see that $\mu_{n-1,1}(\lambda)/\lambda$ ascends monotonously in $(-\infty, 0]$. But, according to Eq. (4.2),

$$\mu'_{n,1}(\lambda) = -\frac{1}{n+1} \left[\frac{\lambda \psi_{n-1,0}(\lambda)}{\psi_{n,0}(\lambda)} \right]^2 \left(\frac{\mu_{n-1,1}(\lambda)}{\lambda} \right)';$$

hence $\mu'_{n,1}(\lambda) < 0$ for every $\lambda < 0$. Thus, $\mu_{n,1}(\lambda)$ descends monotonously in $(-\infty, 0]$ for every $n \geq 1$. Q.E.D.

Now we are able to generalize this result for the entire Padé tableau:

LEMMA 9. *If $\mu_{n,m-1}(\lambda)$ is a one-to-one function, then $\mu_{n,m}(\lambda)$ is one-to-one.*
Proof. We look upon

$$\psi_{n,m}^{(1)}(\lambda) := \psi_{n,m}(\lambda) + \mu_{n,m}(\lambda_0) \psi_{n,m-1}(\lambda).$$

Obviously, $\psi_{n,m}^{(1)}$ is continuous for $\lambda \leq 0$. Moreover,

$$\psi_{n,m}^{(1)}(\lambda) = 0 \Longleftrightarrow R_{n,m}^{(1)}(\lambda) = e^{\lambda}.$$

Thus, $\psi_{n,m}^{(1)}(0) = \psi_{n,m}^{(1)}(\lambda_0) = 0$. Hence, $\psi_{n,m}^{(1)}$ possesses one extremum point in $[\lambda_0, 0]$, at least. We show that there is exactly one such point:

$$\psi_{n,m}^{(1)'}(\lambda) = \psi'_{n,m}(\lambda) + \mu_{n,m}(\lambda_0) \psi'_{n,m-1}(\lambda)$$

$$= \frac{m}{n+m} \psi_{n,m-1}(\lambda) + \mu_{n,m}(\lambda_0) \frac{m-1}{n+m-1} \psi_{n,m-2}(\lambda),$$

and $\psi_{n,m}^{(1)'}(\lambda) = 0$ implies

$$-\frac{\psi_{n,m-1}(\lambda)}{\psi_{n,m-2}(\lambda)} = \frac{n+m}{n+m-1} \times \frac{m-1}{m} \mu_{n,m}(\lambda_0)$$

or

$$\mu_{n,m-1}(\lambda) = \frac{n+m}{n+m-1} \times \frac{m-1}{m} \, \mu_{n,m}(\lambda_0).$$

According to the assumption, $\mu_{n,m-1}$ is one-to-one. Thus, for a certain numerical value

$$\alpha = \frac{n+m}{n+m-1} \times \frac{m-1}{m} \, \mu_{n,m}(\lambda_0) \geqslant 0$$

there exists a unique $\lambda \in (-\infty, 0]$ such that $\mu_{n,m-1}(\lambda) = \alpha$. Therefore, the equation $\psi_{n,m}^{(1)\prime}(\lambda) = 0$ has a unique negative solution. Hence, $\psi_{n,m}^{(1)}(\lambda)$ cuts the negative ray in exactly one point, namely in λ_0.

Let us assume that $\mu_{n,m}(\lambda)$ is not one-to-one in $(-\infty, 0]$. Then $\lambda_1, \lambda_2 < 0$ exist, $\lambda_1 \neq \lambda_2$, such that $\mu_{n,m}(\lambda_1) = \mu_{n,m}(\lambda_2)$. Thus

$$-\frac{\psi_{n,m}(\lambda_1)}{\psi_{n,m-1}(\lambda_1)} = \mu_{n,m}(\lambda_2)$$

or

$$\psi_{n,m}(\lambda_1) + \mu_{n,m}(\lambda_2)\psi_{n,m-1}(\lambda_1) = 0.$$

Hence $\psi_{n,m}^{(1)}(\lambda_1) = 0$, when $\psi_{n,m}^{(1)}$ is fitted to λ_2. But the meaning of fitting is that $\psi_{n,m}^{(1)}(\lambda_2) = 0$. Thus, $\psi_{n,m}^{(1)} = 0$ has two negative solutions, which is evidently a contradiction.

Therefore, $\mu_{n,m}$ is one-to-one. Q.E.D.

Conclusion A. $\mu_{n,m}$ is descending monotonously for every $\lambda \leqslant 0$.

Proof. Clearly, $\mu_{n,m}$ is one-to-one, a conjunction of the Lemmata 8 and 9. But $\mu_{n,m}$ is continuous, $\mu_{n,m}(0) = 0$ and $\mu_{n,m}(\lambda) \geqslant 0$ for $\lambda \leqslant 0$. Therefore, $\mu_{n,m}$ descends monotonously. Q.E.D.

Conclusion B. $\psi_{n,m}^{(1)}(\lambda)$ has exactly two zeros in $(-\infty, 0]$: at the origin and in $\lambda_0 < 0$.

Proof. Repetition of the reasoning which is applied in Lemma 9. Q.E.D.

Apparently, the very definition of $R_{n,m}^{(1)}$ implies that for $\lambda \ll 0$

$$\psi_{n,m}^{(1)}(\lambda) \sim \frac{n!}{(n+m)!} \lambda^m = (-1)^m \frac{n!}{(n+m)!} |\lambda|^m.$$

Thus, for $\lambda \leqslant \lambda_0$ we have $\psi_{n,m}^{(1)}(\lambda)(-1)^m \geqslant 0$ and for $\lambda_0 \leqslant \lambda \leqslant 0$, $\psi_{n,m}^{(1)}(\lambda)(-1)^m \leqslant 0$.

Reformulating this result, we prove

THEOREM 10. *If $R_{n,m}^{(1)}$ is exponentially fitted to $\lambda_0 < 0$, then in $[\lambda_0, 0]$*

$$(-1)^m(R_{n,m}^{(1)}(\lambda) - e^\lambda) \leqslant 0$$

and in $(-\infty, \lambda_0]$,

$$(-1)^m(R_{n,m}^{(1)}(\lambda) - e^\lambda) \geqslant 0,$$

for every $n, m \geqslant 1$.

An immediate conclusion of this theorem is the following lemma:

LEMMA 11. *The pair* $\{R^{(1)}_{n+k,n}, R^{(1)}_{m+l,m}\}$, *when* $0 \leqslant k, l \leqslant 1$, *is dominant if and only if* $n + m$ *is odd.*

This lemma is valid because, according to [2], $R^{(1)}_{n+k,n}, 0 \leqslant k, l \leqslant 1$, is A-stable for every $n \geqslant 1$. If we assume that the Ehle conjecture is valid, namely that $\{R_{n+k,n}, 0 \leqslant k \leqslant 2, 0 \leqslant n\}$ is the set of all A-stable Padé approximations, then Lemma 11 characterizes completely all the dominant pairs which are composed of the approximations $R^{(1)}_{n,m}$.

5. The "Extrapolation" Pairs.

We wish to solve the differential system

$$\dot{x} = f(t, x), \qquad x(t_n) = x_n$$

twice in the interval $[t_n, t_{n+1}]$, by applying an A-stable scheme with the characteristic function χ_1: once with one step of the length $t_{n+1} - t_n$ and once with two steps of the length $\frac{1}{2}(t_{n+1} - t_n)$. According to Section 2, the discussion of the A-stability of a linear combination of the "extrapolants" is reduced into the exploration of the domination property of the pair of appropriate exponential approximations.

Naturally, one is tempted to define $\chi_2(\lambda) = \chi_1^2(\lambda/2)$ and to explore the domination of $\{\chi_1, \chi_2\}$. This approach is, generally speaking, erroneous. If $\chi_1 = R^{(1)}_{n,m}$ and is fitted to λ_0, then $\chi_2(\lambda) = (R^{(1)}_{n,m}(\lambda/2))^2$ is fitted to $2\lambda_0$ and if we combine linearly χ_1 and χ_2, the exponential fitting to λ_0 is lost. Obviously, the proper procedure for the "extrapolation" when $\chi_1(\lambda) = R^{(1)}_{n,m}(\lambda, \mu(\lambda_0))$, is to select

$$\chi_2(\lambda) = (R^{(1)}_{n,m}(\lambda/2, \mu(\lambda_0/2)))^2.$$

Here we define this situation more rigorously:

Definition. When χ is an exponential approximation, we define the set N_χ with the following properties as the *nucleus* of χ:

(a) $N_\chi \subseteq (-\infty, 0] = R^{(-)}$,

(b) $\lambda \in N_\chi$ implies $\chi(\lambda) = \exp(\lambda)$,

(c) $\lambda \in R^{(-)} - N_\chi$ implies $\chi(\lambda) \neq \exp(\lambda)$.

LEMMA 12. *If* χ *is rational and analytical in* $C^{(-)} = \{z \in C: \text{Re } z \leqslant 0\}$ *and is not identically zero, then* N_χ *is finite.*

Proof. If N_χ contains an infinity of points, then it has an accumulation point in $R^{(-)}$ or at $-\infty$.

If this point is finite, then the zeros of the analytical function $\chi(\lambda) - \exp(\lambda)$ have an accumulation point inside the analyticity region $C^{(-)}$. Thus this function is identically zero in $C^{(-)}, \chi(\lambda) \equiv \exp(\lambda)$, which contradicts the rational character of χ.

If the accumulation point of N_χ is $-\infty$ and $\chi = P/Q$, P and Q polynomials, then, obviously, there exists a sequence $\{t_k\}_{k=1}^\infty$, $\lim_{k\to\infty} t_k = -\infty$, such that $P(t_k) = Q(t_k)e^{t_k}$. Hence

$$\lim_{k \to \infty} P(t_k) = \lim_{k \to \infty} Q(t_k)e^{t_k} = 0.$$

Since P is polynomial, $\lim_{t_k \to \infty} P(t_k) = 0$ implies $P(\lambda) \equiv 0$, causing $\chi(z) \equiv 0$ in $C^{(-)}$, which is a contradiction.

Thus, N_χ is finite. Q.E.D.

Definition. We look upon the rational exponential approximation $\chi = \chi(\lambda, s_1, s_2, \ldots, s_q)$, when $s = (s_1, s_2, \ldots, s_q) \in E^q$. If the following requirements:

(a) there exists a $\Omega \subseteq E^q$ so that if $s \in \Omega$, then $\chi(\cdot, s)$ is A-stable;

(b) the number of elements of $N_{\chi(\cdot, s)}$ (which is finite, according to Lemma 12) is invariant for every $s \in \Omega$:

$$N_{\chi(\cdot, s)} \in (-\infty, 0]^p \quad \forall s \in \Omega;$$

(c) for every p-tuple α in $(-\infty, 0]^p$ there exists an $s = s(\alpha) \in \Omega$, so that

$$N_{\chi(\cdot, s)} = \alpha$$

hold, then the approximation χ is *regular*.

The approximations $R_{n,m}$ and $R_{n,m}^{(1)}$ are regular according to the results of the previous sections:

For $R_{n,m}$ it holds:

$$N = \{0\}, \quad \Omega = \varnothing.$$

For $R_{n,m}^{(1)}$ it holds:

$$N = \{0, \lambda_0\}, \quad \Omega = [0, \infty), \quad s_1 = \mu(\lambda_0).$$

Naturally, when we average $\chi(\lambda) = \alpha \chi_1(\lambda) + (1 - \alpha)\chi_2(\lambda)$ we do not want to lose degrees of exponential fitting. Thus, we demand that $N_{\chi_1} = N_{\chi_2}$. Only in this case $N_{\chi_1} = N_{\chi_2} \subseteq N_\chi$ is valid. Thus, when we construct the "extrapolation" pairs, if $\chi_1(\lambda) = \chi_1(\lambda, s(N))$ and χ_1 is regular, we define $\chi_2(\lambda) := (\chi_1(\lambda/2, s(N/2)))^2$. Obviously, in this case, $N_{\chi_2} = N = N_{\chi_1}$.

LEMMA 13. *Assuming that* $N = \{\lambda_1, \lambda_2, \ldots, \lambda_p\}, \lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_p$ *and* χ_1, χ_2 *are defined in the same manner as in the previous paragraph, then:*

(a) *for* $\lambda < \lambda_p, \chi_1(\lambda) > \exp(\lambda)$ *implies that no* λ_0 *exists so that* $\{\chi_1, \chi_2\}$ *is a* λ_0-*dominant pair*;

(b) *for* $\lambda < \lambda_p, \chi_1(\lambda) < \exp(\lambda)$ *implies that a* λ_0 *exists so that* $\{\chi_1, \chi_2\}$ *is a* λ_0-*dominant pair.*

Proof. λ_p is the minimal element of the nucleus N of both χ_1 and χ_2. Thus, either $\chi_1(\lambda) > \exp(\lambda)$ for every $\lambda \in (-\infty, \lambda_p)$ or $\chi_1(\lambda) < \exp(\lambda)$ for every λ in this open interval.

(a) $\chi_1(\lambda) > \exp(\lambda)$ for every $\lambda \in (-\infty, \lambda_p)$. Let us denote $\tilde{\chi}_1(\lambda) = \chi_1(\lambda, s(\frac{1}{2}N))$. Hence $\chi_2(\lambda) = \tilde{\chi}_1^2(\lambda/2)$. $N_{\chi_2} = N$, and thus either $\chi_2(\lambda) > \exp(\lambda)$ for every $\lambda \in (-\infty, \lambda_p)$ or $\chi_2(\lambda) < \exp(\lambda)$.

But $\chi_2(\lambda) = \tilde{\chi}_1^2(\lambda/2) > 0$ and χ_2 is rational. Thus, it is impossible that $0 < \chi_2(\lambda) < \exp(\lambda)$ for every $\lambda \in (-\infty, \lambda_p)$. Hence

$$e^\lambda < \min\{\chi_1(\lambda), \chi_2(\lambda)\}$$

for $\lambda < \lambda_p$ and no $\lambda_0 \leqslant 0$ exists so that $\{\chi_1, \chi_2\}$ is λ_0-dominant.

(b) $\chi_1(\lambda) < \exp(\lambda)$ for every $\lambda \in (-\infty, \lambda_p)$. Two cases are possible: Either $\chi_2(\lambda) > \exp(\lambda)$ for every $\lambda < \lambda_p$ (and then $\chi_1(\lambda) \leqslant \exp(\lambda) \leqslant \chi_2(\lambda)$ for $\lambda \leqslant \lambda_p$ implying that $\{\chi_1, \chi_2\}$ is λ_p-dominant), or there exists a $\xi < \lambda_p$ so that $\widetilde{\chi}_1(\lambda) \leqslant -\exp(\lambda)$ for every $\lambda \leqslant \frac{1}{2}\xi$. ($\frac{1}{2}\lambda_p$ is the smallest element of $N_{\widetilde{\chi}_1}$. The case $\chi_1(\lambda) > \exp(\lambda)$ for $\lambda < \frac{1}{2}\lambda_p$ has been previously discussed. Thus $\widetilde{\chi}_1(\lambda) < \exp(\lambda)$ for $\frac{1}{2}\lambda_p$. If no ξ exists, then there are arbitrarily small points λ for which $|\widetilde{\chi}_1(\lambda)| < \exp(\lambda)$. But $\widetilde{\chi}_1$ is rational and does not vanish identically, because $\widetilde{\chi}_1(\lambda_p/2) = \exp(\lambda_p/2)$ which contradicts the $|\widetilde{\chi}_1(\lambda)| < \exp(\lambda)$ for arbitrarily small points λ.) $\widetilde{\chi}_1(\lambda) \leqslant -\exp(\lambda)$ for $\lambda \in (-\infty, \frac{1}{2}\xi]$ implies that $\chi_2(\lambda) = \widetilde{\chi}_1^2(\lambda/2) > \exp(\lambda)$ for every $\lambda \in (-\infty, \xi]$. Therefore, $\chi_1(\lambda) \leqslant \exp(\lambda) \leqslant \chi_2(\lambda)$ for $\lambda \leqslant \xi$ and $\{\chi_1, \chi_2\}$ is a ξ-dominant pair. Q.E.D.

Conclusion. In the case $\chi_1(\lambda) = R_{n,m}(\lambda)$, $\chi_2(\lambda) = R_{n,m}^2(\lambda/2)$, $R_{n,m}$ A-acceptable and in the case $\chi_1(\lambda) = R_{n,m}^{(1)}(\lambda, \mu(\lambda_0))$, $\chi_2(\lambda) = R_{n,m}^{(1)}(\lambda/2, \mu(\lambda_0/2))^2$, $R_{n,m}^{(1)}$ A-acceptable, a λ^* exists so that $\{\chi_1, \chi_2\}$ is λ^*-dominant if and only if m is odd.

The following lemma indicates that if $N_{\chi_1} = \{0\}$ and the pair of "extrapolants" is λ_0-dominant, it cannot be dominant.

LEMMA 14. *If $N_{\chi_1} = \{0\}$ and $\chi_2(\lambda) = \chi_1^2(\lambda/2)$, then the pair $\{\chi_1, \chi_2\}$ is not dominant.*

Proof. Let us assume that the order of exponential approximation of χ_1 is n. Obviously, this is also the order of approximation of χ_2. If χ is defined as $\chi = \alpha\chi_1 + (1 - \alpha)\chi_2$, then χ is fitted to λ_0 if and only if

$$\alpha = \alpha(\lambda_0) = (e^{\lambda_0} - \chi_2(\lambda_0))/(\chi_1(\lambda_0) - \chi_2(\lambda_0)).$$

But

$$\chi_l(\lambda) = \sum_{k=0}^{n} \frac{1}{k!}\lambda^k + \frac{1}{(n+1)!}a_l\lambda^{n+1} + O(\lambda^{n+2}), \quad l = 1, 2,$$

and $a_l \neq 1$. Thus, applying repetitiously the l'Hôpital rule, we immediately calculate that

$$\alpha(0) = \lim_{\lambda \to 0} \alpha(\lambda) = \frac{1 - a_2}{a_1 \cdot a_2}.$$

Simple calculation verifies that if

$$\chi_1(\lambda) = \sum_{k=0}^{n} \frac{1}{k!}\lambda^k + \frac{1}{(n+1)!}a_1\lambda^{n+1} + O(\lambda^{n+2}),$$

then

$$\chi_1(\lambda/2) = \sum_{k=0}^{n} \frac{1}{k!}(\lambda/2)^k + \frac{1}{(n+1)!}a_1(\lambda/2)^{n+1} + O(\lambda^{n+2})$$

and $\chi_2(\lambda) = \chi_1^2(\lambda/2)$ implies $a_2 = (a_1 - 1)/2^n + 1$ and

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$$\alpha(0) = \frac{1 - a_2}{a_1 - a_2} = \frac{(a_1 - 1)/2^n}{(1 - 1/2^n)(a_1 - 1)}.$$

But $a_1 \neq 1$, thus $\alpha(0) = -1/(2^n - 1) < 0$. If we assume that $\{\chi_1, \chi_2\}$ is a dominant pair, then according to Lemma 2, $\alpha(\lambda) \in [0, 1]$ for every $\lambda \leqslant 0$, which evidently contradicts the negativity of $\alpha(0)$. Therefore, $\{\chi_1, \chi_2\}$ cannot be a dominant pair. Q.E.D.

TABLE 1

λ_0 for λ_0-dominancy of "extrapolated" pairs of the first
λ-dominant Padé approximants $R_{n,m}$

(n, m)	λ_0
$(1, 1)$	-4.7988
$(2, 1)$	-6.9803
$(3, 1)$	-9.1318
$(3, 3)$	-10.0729
$(4, 3)$	-12.0756
$(5, 3)$	-14.2483
$(5, 5)$	-12.2739

TABLE 2

λ_1 for λ_1-dominancy of "extrapolated" pairs of exponentially
fitted Padé approximation $R_{1,1}^{(1)}$, fitted at λ_0

λ_0	$\mu(\lambda_0)$	$\mu(\tfrac{1}{2}\lambda_0)$	λ_1
$-.5$	.090498	.043431	-4.9713
-1.0	.196106	.090498	-5.1557
-2.0	.455697	.196106	-5.5612
-3.0	.779754	.317698	-6.0169
-4.0	1.161296	.455679	-6.5237
-5.0	1.587773	.609920	-7.0820
-10.0	4.002271	1.587773	-10.6213

Lemmata 13 and 14 apparently show that the approach of "extrapolated" pairs is inferior to the approach considered in the previous sections from the stability angle. Nevertheless, this approach is considerably simpler for programming. Moreover, if one applies the error-control technique of halving the step when the estimated error is large, then the approach of "extrapolated" pairs is more natural.

6. The Asymptotic Effect of the Averaging. The numerical distinction between stiff and nonstiff systems of O.D.E.'s at various stages of computation is extremely expensive and not at all practical. Hence, we are interested in good performance of the averaging (1.2) for both stiff and nonstiff systems. The following lemma shows that the averaging has a plausible effect also for nonstiff systems:

LEMMA 15. *If χ_1 and χ_2 are exponential approximations of orders n_1 and n_2, respectively, and*

$$\chi(\mu) = \alpha(\lambda)\chi_1(\mu) + (1 - \alpha(\lambda))\chi_2(\mu), \quad \alpha(\lambda) = (\chi_2(\lambda) - e^\lambda)/(\chi_2(\lambda) - \chi_1(\lambda)),$$

then when λ tends to zero:

(a) $n_1 = n_2$ *implies that the order of χ is $n_1 + 1$.*

(b) $n_1 \neq n_2$ *implies that the order of χ is $\max\{n_1, n_2\}$.*

Proof. Obviously

$$\chi_k(\mu) = \sum_{l=0}^{n_k} \mu^l/l! + a_k \mu^{n_k+1}/(n_k + 1)! + O(\mu^{n_k+2}), \quad k = 1, 2.$$

Thus:

(a) If $n_1 = n_2$ then, by the same reasoning as in Lemma 14,

$$\alpha(0) = (a_2 - 1)/(a_2 - a_1).$$

(b) If $n_1 < n_2$, then $\chi_2 - \exp(\mu)$ has at the origin a zero of a greater order than $\chi_2 - \chi_1$, implying that $\alpha(0) = 0$.

(c) If $n_1 > n_2$, then both the numerator $\chi_2 - e^\mu$ and the denominator $\chi_2 - \chi_1$ tend at the origin to $\chi_2(0) = 1$, thus $\alpha(0) = 1$.

Therefore, if $n_1 \neq n_2$ and λ tends to zero, then the order of χ is $\max\{n_1, n_2\} = n_p$ and $\chi \equiv \chi_p$. On the other hand, if $n_1 = n_2$, then when λ approaches zero,

$$\chi(\mu) = \sum_{l=0}^{n_1} \mu^l/l! + \frac{1}{(n_1 + 1)!}\left[a_1\frac{a_2 - 1}{a_2 - a_1} + a_2\left(1 - \frac{a_2 - 1}{a_2 - a_1}\right)\right]\mu^{n_1+1}$$

$$+ O(\mu^{n_1+2}) = \sum_{l=0}^{n_1+1} \mu^l/l! + O(\mu^{n_1+2});$$

and the order is increased. Q.E.D.

Lemma 15 hints about an asymptotic connection between the averaging (1.2) and the conventional polynomial extrapolation. The paper [4] gives more specific results on this subject, concerning the scheme

(6.1) $$\chi(\mu) = \sum_{k=1}^{n-1} \alpha_k \chi_k(\mu) + \left(1 - \sum_{k=1}^{n-1} \alpha_k\right)\chi_n(\mu),$$

when $\chi_k(\mu) = ((k + \mu/2)/(k - \mu/2))^k$ is the characteristic function of the trapezoidal rule which is applied with k substeps. It is shown in [4] that the scheme (6.1) can be

exponentially fitted to λ_k, $1 \leqslant k \leqslant N - 1$. The following result is proved in [4] and is given here without proof:

LEMMA 16. *If $F(\lambda_1, \lambda_2, \ldots, \lambda_{N-1})$ is the space of all the n-tuples $(\alpha_1, \alpha_2, \ldots, \alpha_N)$, $\alpha_N = 1 \cdot \Sigma_{k=1}^{N-1} \alpha_k$, which fits the scheme (6.1) to λ_k, $1 \leqslant k \leqslant N - 1$, and*

$$F_0 = \lim_{\lambda_i \to 0\,;\,1 \leqslant i \leqslant N-1} (\lambda_1, \lambda_2, \ldots, \lambda_{N-1}), \quad \textit{if } \mathbf{a}^{(l)} = (a_1^{(l)}, a_2^{(l)}, \ldots, a_N^{(l)})$$

are the coefficients of the lth order odd-power Romberg extrapolation [5] of the trapezoidal rule, then,

$$F_0 = \mathrm{Sp}\{\mathbf{a}^{(1)}, \mathbf{a}^{(2)}, \ldots, \mathbf{a}^{(N-1)}\}.$$

7. Conclusions and Suggestions for Further Research.
Translating the results of this paper from the nomenclature of the dominating pairs into the language of A-stability, we can conclude that:

(a) The scheme (1.2) for $\chi_1 = R_{n_1, m_1}$, $\chi_2 = R_{n_2, m_2}$ or $\chi_1 = R_{n_1, m_1}^{(1)}$, $\chi_2 = R_{n_2, m_2}^{(1)}$ can be exponentially fitted with preservation of A-acceptability if $m_1 + m_2$ is odd. If $\chi_1 = R_{n_1, n_1}$, $\chi_2 = R_{n_2, n_2}$ (and, thus $|R_{n_1, n_1}(it)| \equiv |R_{n_2, n_2}(it)| \equiv 1$ for every $t \in (-\infty, \infty)$), then χ is A-acceptable if and only if $n_1 + n_2$ is odd.

(b) The scheme (1.2) for χ_1 and χ_2 which are "extrapolants" cannot be A-acceptably fitted to every $\lambda \leqslant 0$. In certain cases a $\lambda_0 < 0$ exists so that it can be A-acceptably fitted to every $\lambda \leqslant \lambda_0$.

(c) Even if the differential system is nonstiff, we benefit from the averaging, which behaves asymptotically as extrapolation.

This paper does not exhaust, by any means, the subject of A-stability in its connection to the averaged schemes of type (1.2). There are several "natural" suggestions for further research:

(1) Domination tests for other pairs of exponential approximations. The first candidate for such tests is the doubly-fitted approximation considered by Ehle and Picel [3] and by Nørsett [6]:

$$R_n^{(2)} := \frac{(1 - \mu_1 - \mu_2)P_{n,n} + \mu_1 P_{n,n-1} + \mu_2 P_{n,n-2}}{(1 - \mu_1 - \mu_2)Q_{n,n} + \mu_1 Q_{n,n-1} + \mu_2 Q_{n,n-2}}$$

which is A-acceptable when fitted to two arbitrary negative arguments.

(2) Consideration of averages of more than two exponential approximations and their A-acceptability. This subject seems to be extremely complicated and even in the simple case considered in [4] no remarkable results have been achieved.

(3) Closer observation of the asymptotic behavior of the averaging, when the fitting argument tends to zero. It is interesting whether the behavior of the trapezoidal rule, as exhibited in Lemma 16, is characteristic to this scheme or represents more general phenomena.

Department of Mathematics
Ben-Gurion University
Beersheba, Israel

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