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TWO-POINT PADÉ APPROXIMANTS FOR STIELTJES FUNCTIONS AND THEIR APPLICATION TO COMPOSITE MATERIALS

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By employing special continued fractions to asymptotic expansions at zero and infinity, the convergence of the balanced and unbalanced two-point Padé approximants (2PPA) to a Stieltjes function is studied in a real domain. We prove that certain balanced and unbalanced two-point Padé approximants form a monotone sequence of upper and lower bounds uniformly converging to a Stieltjes function. The observed monotone and uniform convergence of 2PPA is exemplified in the evaluation of bounds on the effective transport coefficients of periodic inhomogeneous media.

1. Introduction

The mathematical properties of one-point Padé approximants to a series of Stieltjes functions have been extensively investigated in the past two decades by Baker (1975), Baker and Graves-Morris (1981a, 1981b), Bultheel (1987), Gilewicz (1978), Jones and Thron (1980), and Wall (1948). In particular, necessary and sufficient conditions for a monotone and uniform convergence of one-point Padé approximants constructed for Stieltjes functions were established, cf. Thms. 16.1–16.3 in (Baker, 1975).

On the other hand, two-point Padé approximants (2PPA) to Stieltjes functions represented by power series developed at zero and infinity have not been examined as thoroughly as the one-point Padé ones. The studies reported in the relevant literature by González-Vera and Njåstad (1990), Gragg (1980), Jones *et al.* (1983) and Jones and Thron (1970) are concerned mainly with 2PPA having the same number of coefficients of power expansions at zero and infinity (a balanced situation). A 2PPA with finite, non-equal numbers of coefficients of two formal series of Taylor and Laurent types has been investigated by Tokarzewski *et al.* (1994a, 1994b) and Tokarzewski (1996). Some special 2PPA was examined by Casasús and González-Vera (1985). Recently, the problem of estimating the exact rate of the convergence of 2PPA to a Stieltjes-type function has been solved by Lagomasino and Finkelshtein (1995). A method of interpolation of a Carathéodory function by means of some modified approximants was proposed by Bultheel *et al.* (1995).

In the present work, the convergence of both balanced and unbalanced, two-point Padé approximants to asymptotic expansions of a Stieltjes function at zero and at

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infinity is studied. An application of the results to the theory of composite materials is also given.

The paper is organized as follows: In Section 2, we introduce basic definitions, notations and assumptions concerning Stieltjes functions and diagonal two-point Padé approximants. In Section 3, we recall the results regarding one-point Padé approximants, important for our further developments. In Section 4, special continued-fraction representations of two-point Padé approximants are derived. Some basic inequalities for 2PPA are discussed in Section 5. In Section 6, the uniform and monotone convergence of two-point Padé approximants to a Stieltjes function is proved. The general recurrence formulae for finding two-point Padé approximants are given in Sections 7 and 8. In Sections 9 and 10, numerical examples illustrating the theoretical results are presented. The last section summarizes the achieved results.

2. Preliminaries and Basic Notions

We consider a Stieltjes function $xf_1(x)$ defined for $0 < x < \infty$ by means of the following Stieltjes integral:

$$xf_1(x) = x\int_0^\infty \frac{\mathrm{d}\gamma_1(u)}{1+xu} \tag{1}$$

The spectrum $\gamma_1(u)$ ($\gamma(u)$ in the relevant paper (Tokarzewski *et al.*, 1994b)) is a real and non-decreasing function defined for $0 \le u \le \infty$ and such that the asymptotic expansion of $xf_1(x)$ at $x = 0$ satisfies Carleman's criterion

$$xf_1(x) \simeq \sum_{n=1}^{\infty} c_n x^n, \qquad \sum_{n=1}^{\infty} c_n^{-1/2n} = \infty \tag{2}$$

where the coefficients

$$c_n = (-1)^{n+1}\int_0^\infty u^{n-1}\,\mathrm{d}\gamma_1(u) \tag{3}$$

are finite. The second of Carleman's conditions (2) is sufficient for the convergence of a sequence of one-point Padé approximants to the Stieltjes function (1), see Theorem 5.5.1 in (Baker and Graves-Morris, 1981a).

The asymptotic expansion of $xf_1(x)$ at $x = \infty$ takes the form

$$xf_1(x) \simeq \sum_{n=1}^{\infty} C_n(1/x)^{n-1} \tag{4}$$

As previously, we assume that the moments

$$C_n = (-1)^{n+1}\int_0^\infty u^{-n}\,\mathrm{d}\gamma(u), \qquad n = 1,2,\dots \tag{5}$$

are finite and satisfy Carleman's criterion.

The diagonal two-point Padé approximants for series (2) and (4) have the following general form:

$$[M/M]_k(x) = \frac{a_{1k}x + a_{2k}x^2 + \cdots + a_{Mk}x^M}{1 + b_{1k}x + b_{2k}x^2 + \cdots + b_{Mk}x^M}, \qquad 0 \le k \le 2M \tag{6}$$

Let us consider now the power expansion of (6) at zero

$$[M/M]_k(x) = \sum_{n=1}^{\infty} c_{nk}x^n \tag{7}$$

and infinity

$$[M/M]_k(x) = \sum_{n=1}^{\infty} C_{nk}(1/x)^{n-1} \tag{8}$$

By definition, the rational function (6) is the two-point Padé approximant $[M/M]_k(x)$ to Stieltjes function (1) if

$$c_{nk} = c_n \quad \text{for} \quad n = 1, 2, \ldots, p, \qquad p = 2M - k \tag{9}$$

and

$$C_{nk} = C_n \quad \text{for} \quad n = 1, 2, \ldots, k \tag{10}$$

According to (9) and (10), the Padé approximant $[M/M]_k(x)$ given by (6) matches p coefficients of the series (2) and k coefficients of the series (4), where $p + k = 2M$. Hence $[M/M]_0(x)$ and $[M/M]_{2M}(x)$ stand for the one-point Padé approximants to the Stieltljes series (2) and (4), respectively.

Multiplying both sides of (1), (4) and (2) by $s = 1/x$, we arrive at the Stieltjes function

$$f_1(x) = \int_0^{\infty} \frac{\mathrm{d}\gamma_1(u)}{1 + xu} = s\phi_1(s) = s\int_0^{\infty} \frac{\mathrm{d}\gamma_1(u)}{s + u}, \quad s = 1/x \tag{11}$$

with power expansions

$$f_1(x) \simeq \sum_{n=1}^{\infty} C_n s^n, \quad s = 1/x \tag{12}$$

$$f_1(x) \simeq \sum_{n=1}^{\infty} c_n (1/s)^{n-1}, \quad s = 1/x \tag{13}$$

at $s = 0$ and $s = \infty$, respectively.

By comparing (2) with (12) and (4) with (13) we conclude that the two-point Padé approximants $[M/M]_k(x)$ to (2) and (4) can be obtained from those $[M/M]_p(s)$ to (12) and (13) by means of the following important identity:

$$[M/M]_k(x) = x[M/M]_p(s), \quad s = 1/x, \quad p = 2M - k \tag{14}$$

Therefore general recurrence formulae for evaluation of $[M/M]_p(s)$ for (12) can be obtained from algorithms computing $[M/M]_k(x)$ for (2) and (4) by replacing c_n by C_n,p by k and x by s.

3. One-Point Padé Approximants $[M/M]_0$

We start by recalling some most important results for one-point Padé approximants $[M/M]_0(x)$ to the Stieltjes function $xf_1(x)$ defined by (1), indispensable for our further investigations:

1) $[M/M]_0(x)$ has the continued fraction representation of type S (Baker, 1975; Baker and Graves-Morris, 1981b):

$$[M/M]_0(x) = \frac{xe_1}{1} + \frac{xe_2}{1} + \cdots + \frac{xe_{2M-1}}{1} + \frac{xe_{2M}}{1} \tag{15}$$

2) The coefficients of the continued fraction (15) are positive,

$$e_n > 0, \qquad n = 1, 2, \ldots, 2M \tag{16}$$

3) For each real and non-negative x, the Padé approximants $[M/M-1]_0(x)$ and $[M/M]_0(x)$, $M = 1, 2, \ldots$ form monotone sequences of upper and lower bounds on $xf_1(x)$:

$$\begin{aligned}[M/M-1]_0(x) &\geq [M+1/M]_0(x) \geq xf_1(x) \\ &\geq [M+1/M+1]_0(x) \geq [M/M]_0(x)\end{aligned} \tag{17}$$

4) The bounds $[M+1/M]_0(x)$ and $[M+1/M+1]_0(x)$ converge uniformly to $xf_1(x)$ on compact subsets of $(0, \infty)$:

$$\lim_{M\to\infty} [M+1/M]_0(x) = \lim_{M\to\infty} [M/M]_0(x) = xf_1(x) \tag{18}$$

5) If $f_j(x)$ is a Stieltjes function defined by a spectrum $\gamma_j(u)$, then $f_{j+1}(x)$ is also a Stieltjes function with the spectrum $\gamma_{j+1}(u)$, provided that (Baker, 1975, Lemma 15.3)

$$f_j(x) = \frac{f_j(0)}{1 + xf_{j+1}(x)}, \quad x > 0 \tag{19}$$

4. Continued-Fraction Representation for $xf_1(x)$

In this section, some special continued-fraction representations for the two-point Padé approximants $[M/M]_k(x)$ to series (2) and (4) will be derived. To this end, we introduce the family of Stieltjes functions $f_{j+1}(x)(j = 0, 1, \ldots)$

$$f_{j+1}(x) = C^{(j+1)} + \int_0^\infty \frac{\mathrm{d}\gamma_{j+1}(u)}{1 + xu} \tag{20}$$

interrelated by the following fractional transformation:

$$f_{j+1}(x) = \frac{f_{j+1}(0)}{1 + x f_{j+2}(x)}, \qquad j = 0, 1, \ldots, \qquad x > 0 \tag{21}$$

with $f_1(x)$ given by (1), where $C^{(1)} = 0$. Note that the constants $C^{(j+1)}(j = 1, 2, \ldots)$ are uniquely determined by the transformation (21) applied j times to the asymptotic expansions (2) and (4). For instance, from (2), (4) and (21), it follows immediately that $C^{(1)} = 0$, $C^{(2)} = c_1/C_1 > 0$, $C^{(3)} = 0, \ldots$. Hence, in general, we have

$$C^{(j+1)} = 0 \quad \text{for} \quad j = 0, 2, \ldots, \qquad C^{(j+1)} > 0 \quad \text{for} \quad j = 1, 3, \ldots \tag{22}$$

By choosing $x = 1/s$ in (20) one obtains

$$f_{j+1}(x) = f_{j+1}(1/s) = s\phi_{j+1}(s), \quad j = 0, 1, \ldots, \quad x > 0 \tag{23}$$

where

$$s\phi_{j+1}(s) = C^{(j+1)} + s\int_0^\infty \frac{\mathrm{d}\Gamma_{j+1}(\tau)}{1 + s\tau}, \quad \mathrm{d}\Gamma_{j+1}(\tau) = -\tau \mathrm{d}\gamma_{j+1}(1/\tau) \tag{24}$$

Remark 1. The Stieltjes functions $f_{j+1}(x)$ defined by (20)–(22) and Stieltjes functions $s\phi_{j+1}(s)$ appearing in (23)–(24) are equivalent, provided $s = 1/x$.

We now turn to the derivation of a special continued-fraction representation for the Stieltjes function $xf_1(x)$. Applying (19) to $xf_1(x)\, p$ times, we obtain

$$xf_1(x) = \frac{xg_1}{1} + \frac{xg_2}{2} + \cdots + \frac{xg_p}{1 + xf_{p+1}(x)}, \quad g_n = f_n(0), \quad n = 1, 2, \ldots, p \tag{25}$$

Here the coefficients $g_n > 0$ are uniquely determined by a given number of p coefficients of the power series (2). According to (23) and (24), we have

$$f_{p+1}(x) = s\phi_{p+1}(s) = C^{(p+1)} + s\int_0^\infty \frac{\mathrm{d}\Gamma_{p+1}(\tau)}{1 + s\tau}, \qquad s = 1/x \tag{26}$$

where $C^{(p+1)}$ are still defined by (21). The Stieltjes functions $s\phi_{p+1}(s)$ determined by (26) have the following continued-fraction representations which depend on whether $C^{(p+1)} > 0$ or $C^{(p+1)} = 0$ (Baker and Graves-Morris, 1981b, p.127, (5.1), (5.5)):

$$s\phi_{p+1}(s) = \begin{cases} C^{(p+1)} + \dfrac{sg_{p+2}}{1} + \cdots + \dfrac{sg_{2M}}{1 + s\phi_{2M+1}(s)} & \text{if } p = 1, 3, \ldots \\ \dfrac{sg_{p+1}}{1} + \cdots + \dfrac{sg_{2M}}{1 + s\phi_{2M+1}(s)} & \text{if } p = 2, 4, \ldots \end{cases} \tag{27}$$

The positive coefficients $C^{(p+1)}$ and $g_{p+j}\,(j = 1, 2, \ldots, k)$ are uniquely determined by k coefficients of (4) and p parameters $g_n\,(n = 1, 2, \ldots, p)$ of (25). Substituting (27) into (25) and setting $C^{(p+1)} = g_{p+1}$, we obtain a special continued-fraction representation for $xf_1(x)$ in the form

$$xf_1(x) = \begin{cases} \dfrac{xg_1}{1} + \cdots + \dfrac{xg_p}{1 + xg_{p+1}} + \dfrac{g_{p+2}}{1} + \dfrac{sg_{p+3}}{1} \\ \qquad + \cdots + \dfrac{sg_{2M}}{1 + s\phi_{2M}(s)} & \text{if } p \text{ is odd} \\ \dfrac{xg_1}{1} + \cdots + \dfrac{xg_p}{1} + \dfrac{g_{p+1}}{1} + \dfrac{sg_{p+2}}{1} \\ \qquad + \cdots + \dfrac{sg_{2M}}{1 + s\phi_{2M+1}(s)} & \text{if } p \text{ is even} \end{cases} \tag{28}$$

where $s = 1/x$. By dividing the right-hand side of (28) by $x = 1/s$ and replacing g, p, x by d, k, s, respectively, we arrive at an equivalent continued-fraction representation for $xf_1(x)$, namely

$$xf_1(x) = \begin{cases} \dfrac{d_1}{1} + \dfrac{sd_2}{1} + \cdots + \dfrac{sd_k}{1 + sd_{k+1}} + \dfrac{d_{k+2}}{1} + \dfrac{xd_{x+3}}{1} \\ \qquad + \cdots + \dfrac{xd_{2M}}{1 + xf_{2M+1}(x)} & \text{if } k \text{ is odd} \\ \dfrac{d_1}{1} + \dfrac{sd_2}{1} + \cdots + \dfrac{sd_k}{1} + \dfrac{d_{k+1}}{1} + \dfrac{xd_{k+2}}{1} \\ \qquad + \cdots + \dfrac{xd_{2M}}{1 + xf_{2M+1}(x)} & \text{if } k \text{ is even} \end{cases} \tag{29}$$

The continued fraction (29) can also be derived by applying the procedure given by (20)–(28), to the asymptotic expansions (12) and (13). All the coefficients g_n and d_n $(n = 1, 2, \ldots, p + k)$ appearing in (28) and (29) are positive, i.e.

$$g_n > 0, \quad d_n > 0, \qquad n = 1, 2, \ldots, 2M = p + k \tag{30}$$

From (27) and (28), we conclude immediately the special continued-fraction representations for two-point Padé approximants defined by (6)–(10). For $s = 1/x$ and $k + p = 2M$ we have

$$[M/M]_{2M-p}(x) = \begin{cases} \dfrac{xg_1}{1} + \cdots + \dfrac{xg_p}{1 + xg_{p+1}} + \dfrac{g_{p+2}}{1} + \dfrac{sg_{p+3}}{1} \\ \qquad + \cdots + \dfrac{sg_{2M}}{1} & \text{if } p \text{ is odd} \\ \dfrac{xg_1}{1} + \dfrac{xg_p}{1} + \dfrac{g_{p+1}}{1} + \dfrac{sg_{p+2}}{1} + \cdots + \dfrac{sg_{2M}}{1} & \text{if } p \text{ is even} \end{cases} \tag{31}$$

and

$$
[M/M]_k(x) = \begin{cases} \dfrac{d_1}{1} + \dfrac{sd_2}{1} + \dots + \dfrac{sd_k}{1 + sd_{k+1}} + \dfrac{d_{k+2}}{1} + \dfrac{xd_{k+3}}{1} \\ \qquad + \dots + \dfrac{xd_{2M}}{1} & \text{if } p \text{ is odd} \\ \dfrac{d_1}{1} + \dfrac{sd_2}{1} + \dots + \dfrac{sd_k}{1} + \dfrac{d_{k+1}}{1} + \dfrac{xd_{k+2}}{1} \\ \qquad + \dots + \dfrac{xd_{2M}}{1} & \text{if } p \text{ is even} \end{cases} \tag{32}
$$

It is worth noticing that $[M/M]_{2M-p}(x) = [M/M]_k(x)$ if $p + k = 2M$. In the next section, some basic inequalities for two-point Padé approximants $[M/M]_{2M-p}(x)$ and $[M/M]_k(x)$ are derived.

5. Basic Inequalities for $[M/M]_{2M-p}$ and $[M/M]_k$

To simplify the notation for $[M/M]_{2M-p}(x)$ and $[M/M]_k(x)$ given by (31) and (32), it is convenient to introduce the following continued-fraction operator:

$$
G_{n+1,y}^{n+m} f = \begin{cases} \dfrac{g_{n+1}}{1} + \dfrac{yg_{n+2}}{1} + \dots + \dfrac{yg_{n+m}}{1} + \dfrac{yf}{1} & \text{if } n = 0, 2, \dots \\ g_{n+1} + \dfrac{yg_{n+2}}{1} + \dots + \dfrac{g_{n+m}}{1} + \dfrac{yf}{1} & \text{if } n = 1, 3, \dots \end{cases} \tag{33}
$$

where $y = x$ or $y = s$, $s = 1/x$. On account of (33), the relations (28), (29) and (31), (32) take the following forms:

$$
xf_1(x) = xG_{1,x}^p G_{p+1,s}^{2M} \phi_{2M+1}(s) = G_{1,s}^k G_{k+1,x}^{2M} f_{2M+1}(x) \tag{34}
$$

$$
[M/M]_{2M-p}(x) = xG_{1,x}^p G_{p+1,s}^{2M} 0, \quad [M/M]_k(x) = G_{1,s}^k G_{k+1,x}^{2M} 0 \tag{35}
$$

Now we are in a position to write down the inequalities valid for two- point Padé approximants $xG_{1,x}^p G_{p+1,s}^{2M} 0$ and $G_{1,s}^k G_{k+1,x}^{2M} 0$:

$$
(-1)^p xG_{1,x}^{p-1} 0 > (-1)^p xG_{1,x}^p G_{p+1,s}^{2M} 0 > (-1)^p xG_{1,x}^p 0 \tag{36}
$$

$$
(-1)^k G_{1,s}^{k-1} 0 > (-1)^k G_{1,s}^k G_{k+1,x}^{2M} 0 > (-1)^k G_{1,s}^k 0 \tag{37}
$$

and

$$
(-1)^p xG_{1,x}^p G_{p+1,s}^{2M} 0 < (-1)^p xG_{1,x}^p G_{p+1,s}^{2M+2} 0 \tag{38}
$$

$$
(-1)^k G_{1,s}^k G_{k+1,x}^{2M} 0 < (-1)^k G_{1,s}^k G_{k+1,x}^{2M+2} 0 \tag{39}
$$

where $0 < x < \infty$, $s = 1/x$. The inequalities (36)–(39) are a direct consequence of the inequalities (30) and the simple recurrence relations for the C- and S-continued fractions of the type $G^j_{1,y}0$ appearing in (36)–(39) (Baker and Graver-Morris, 1981a, Chap.4).

To discuss the formulae (36) and (37), let us note that $xG^p_{1,x}0 = xG^{2M-k}_{1,x}0$ are the one-point Padé approximants to the p coefficients of the series (2), as $G^k_{1,s}0 = G^{2M-p}_{1,s}0$ are to the k terms of the expansion (4). Both $xG^{2M-k}_{1,s}0$ (k is fixed) and $G^{2M-p}_{1,s}0$ (p is fixed) converge to $xf_1(x)$ as $M \to \infty$, cf. Carleman's criterion assumed for asymptotic expansions (2) and (4). Thus we have

$$\lim_{M\to\infty}[M/M]_{2M-p}(x) = xf_1(x), \qquad \lim_{M\to\infty}[M/M]_k = xf_1(x) \tag{40}$$

Remark 2. For a fixed p the two-point Padé approximants $[M/M]_{2M-p}(x)$ and for a fixed k the $[M/M]_k(x)$ converge to the Stieltjes function $xf_1(x)$ for $x \in (0,\infty)$ as $M \to \infty$.

The relations (38) and (39) combined with (40) yield

$$(-1)^{k(M+1)}[M+1/M+1]_{k(M+1)}(x) > (-1)^{k(M)}[M/M]_{k(M)}(x), \quad x > 0 \tag{41}$$

$$(-1)^{k(M)}xf_1(x) > (-1)^{k(M)}[M/M]_{k(M)}(x), \quad x > 0 \tag{42}$$

where $k(M)$ is given by

$$k(M) = \begin{cases} 2M - p & \text{if } p \text{ is fixed} \\ k & \text{if } k \text{ is fixed} \end{cases} \tag{43}$$

Remark 3. For $x > 0$ the inequalities (42) provide the best estimates for the Stieltjes functions $xf_1(x)$ with respect to given numbers of coefficients of the asymptotic expansions of $xf_1(x)$ at $x = 0$ and at $x = \infty$.

6. Convergence of $[M_n/M_n]_{k(M_n)}$ and $[M_n/M_n]_{k(M_n)}$ to $xf_1(x)$

Now we are prepared to study the general case of the two-point Padé approximants $[M_n/M_n]_{k(M_n)}$ to $xf_1(x)$ given by (1)–(5). For that purpose, we assume that M_n is a monotone sequence of natural numbers and $k(M_n)$ stands for a monotone sequence of either odd or even natural numbers, where $n = 1, 2, \ldots$.

Theorem 1. *Let $k(M_n)\,(n = 1, 2, \ldots)$ be a monotone sequence of even or odd natural numbers satisfying the inequalities*

$$2(M_{n+1}) - 2(M_n) \geq k(M_{n+1}) - k(M_n), \quad 2M_n \geq k(M_n) \tag{44}$$

Then any sequences of two-point Padé approximants $[M_n/M_n]_{k(M_n)}$ to asymptotic expansions of a Stieltjes function defined by (1)–(5) converge to $xf_1(x)$

$$\lim_{n\to\infty}[M_n/M_n]_{k(M_n)} = xf_1(x) \tag{45}$$

and for $x > 0$ they obey the following fundamental inequalities:

$$(-1^{k(M_n)}[M_n/M_n]_{k(M_n)} < (-1)^{k(M_{n+1})}[M_{n+1}/M_{n+1}]_{k(M_{n+1})} \tag{46}$$

$$(-1)^{k(M_n)}[M_n/M_n]_{k(M_n)} < (-1)^{k(M_n)}xf_1(x) \tag{47}$$

as $n \to \infty$. The relations (45)–(47) imply that the Padé approximants $[M_n/M_n]_{k(M_n)}$ form monotone sequences of upper (if $k(M_n)$'s are odd) and lower (if $k(M_n$'s are even) bounds converging uniformly to $xf_1(x)$ in compact subsets of $(0,\infty)$.

Proof. Let us assume that $k(M_n)\,(n = 1, 2, \dots)$ is a sequence of even natural numbers only (for odd numbers the proof is analogous). We start from the two-point Padé approximant identity

$$[M_n/M_n]_{k(M_n)} = [M_n/M_n]_{2M_n - p(M_n)} \tag{48}$$

where $2M_n = p(M_n) + k(M_n)$. If $k(M_n)$ is fixed, then by increasing $p(M_n)$ to $p(M_{n+1})$ we arrive at

$$[M_{n(n+1)}/M_{n(n+1)}]_{k(M_n)} = [M_{n(n+1)}/M_{n(n+1)}]_{2M_{n(n+1)} - p(M_{n+1})} \tag{49}$$

where $2M_{n(n+1)} = [k(M_n) + p(M_{n+1})]$. From (41)–(43) we deduce that

$$[M_n/M_n]_{k(M_n)} < [M_{n(n+1)}/M_{n(n+1)}]_{k(M_n)} \tag{50}$$

Conversely, keeping $p(M_{n+1})$ fixed we increase $k(M_n)$ to $k(M_{n+1})$, cf. the assumption (44). On the basis of the identity

$$[M_{n+1}/M_{n+1}]_{2M_{n+1} - p(M_{n+1})} = [M_{n+1}/M_{n+1}]_{k(M_{n+1})} \tag{51}$$

from (41)–(43) and (50), (51), it follows that

$$[M_n/M_n]_{k(M_n)} < [M_{n+1}/M_{n+1}]_{k(M_{n+1})} \tag{52}$$

Analogously, for an odd $k(M_n)\,(n = 1, 2, \dots)$ we obtain

$$[M_n/M_n]_{k(M_n)} > [M_{n+1}/M_{n+1}]_{k(M_{n+1})} \tag{53}$$

On account of (52) and (53), the inequalities (46) are established.

To prove the convergence of $[M_n/M_n]_{k(M_n)(x)}$ to $xf_1(x)$, let us note that for $x > 0$ we have

$$(-1)^{p(n)}xG_1^{p(n)-1}0 > (-1)^{p(n)}xG_1^{p(n)}xG_{p+1,s}^{2M(n)}0 > (-1)^{p(n)}xG_{1,x}^{p(n)}0 \tag{54}$$

where we have introduced $p(n) = p(M_n)$. Since one-point Padé approximants $xG_{1,x}^{p(n)}$ appearing in (54) converge to $xf_1(x)$, the two-point Padé approximants $[M_n/M_n]_{k(M_n)}(x)$ also converge to $xf_1(x)$, cf. (44). ■

A direct consequence of Theorem 1 is the following remark useful for practical applications:

Remark 4. The bounds $[M_n/M_n]_{k(M_n)}$ are obtained using $2M_n - k(M_n)$ coefficients of the series (2) and $k(M_n)$ coefficients of the series (4). The use of additional coefficients (cf. (44)) improves these bounds.

Theorem 1 is the main theoretical result of the present paper, since it solves the problem of the monotone and uniform convergence of both balance and unbalanced two-point Padé approximants to a Stieltjes function $xf_1(x)$ defined by (1)–(5). It is worth noticing that for the particular cases defined by: (i) $M_n = n = M$ and $k(M) = M$; (ii) $M_n = n = M$ and $k(M) = 1, 2$; (iii) $M_n = n = M$ and $K(M) = 0$ the fundamental inequalities (45) and (46) reduce to the results reported earlier by (i) González-Vera and Njåstad (1990, Th.2.3); (ii) Tokarzewski *et al.* (1994b, Thms. 1 and 2); (iii) Baker (1975, Thm. 15.2), respectively.

In Sections 7 and 8, a general algorithm for evaluation of two-point Padé approximants to the asymptotic expansions of Stieltjes functions at zero and infinity will be constructed.

7. Basic Equation for the Continued-Fraction Parameters g_n

In the first step, we derive a system of equations for determination of the coefficients g_n of continued fractions (31). We assume that p terms of the power series (2) and k terms of the power expansion (4) are available. Hence

$$xf_1(x) \sim \sum_{n=1}^{p} c_n^{(1)} x^n, \qquad xf_1(x) \sim \sum_{n=1}^{k} C_n^{(1)} (1/x)^{n-1} \tag{55}$$

The linear fractional transformation (22) applied to (55) p times leads to the system of algebraic equations

$$\sum_{n=1}^{p-j+1} c_n^{(j)} x^n = \frac{x c_1^{(j)}}{1 + \sum_{n=1}^{p-1} c_n^{(j+1)} x^n}, \quad j = 1, 2, \ldots, p \tag{56}$$

which determines the unknown coefficients $g_j = c_1^{(j)}$ $(j = 1, 2, \ldots, p)$. Note that in (56) we have

$$\sum_{n}^{k} e_n = 0 \quad \text{if } p < k \tag{57}$$

The next step is to find k coefficients $C_n^{(p+1)}$ $(n = 1, 2, \ldots, k)$ of the power expansion of $xf_{p+1}(x)$ at $s = 0$, i.e.

$$xf_{p+1}(x) \sim \sum_{n=1}^{k} C_n^{(p+1)} s^{n-1}, \qquad s = 1/x \tag{58}$$

from k terms of the expansion of $xf_1(x)$, i.e.

$$xf_1(x) \sim \sum_{n=1}^{k} C_n^{(1)} s^{n-1}, \qquad s = 1/x \tag{59}$$

By substituting (55) and (58) into (25), for $x = 1/s$ we obtain the system of equations which enables us to determine the coefficients $C_n^{(p+1)}$ $(n = 1, 2, \ldots, k)$:

$$\begin{cases} \sum_{n=1}^{k} C_n^{(1)} s^{n-1} = \frac{g_1}{s} + \frac{g_2}{1} + \cdots + \frac{g_p}{\alpha + \sum_{n=1}^{k} C_n^{(p+1)} s^{n-1}} \\ \alpha = \begin{cases} 1, & \text{if } p \text{ is odd} \\ s, & \text{if } p \text{ is even} \end{cases} \end{cases} \tag{60}$$

Now we can construct an S-continued fraction to (55). On account of (26) and (27), the recurrence equations determining the coefficients $g_{p+j} = C_1^{(p+j)}$ $(j = 1, 2, \ldots, k)$ are as follows:

(i) If p is even, then

$$\sum_{n=1}^{k-j+1} C_n^{(p+j)} s^n = \frac{sC_1^{(p+j)}}{1 + \sum_{n=1}^{k-j} C_n^{(p+j+1)} s^n}, \quad j = 1, 2, \ldots, k \tag{61}$$

(ii) If p is odd, then

$$\sum_{n=2}^{k-j+1} C_n^{(p+j)} s^{n-1} = \frac{sC_2^{(p+j)}}{1 + \sum_{n=2}^{k-j} C_n^{(p+j+1)s^n}}, \quad j = 1, 2, \ldots, k-1 \tag{62}$$

The formulae (55)–(62) allow us to find the parameters g_k $(n = 1, 2, \ldots, k + p)$ from given p coefficients of the power series (2) and k coefficients of the power expansion (4).

8. Recurrence Formulae for the Continued-Fraction Parameters g_n

This section deals with some algorithms for the determination of parameters g_n $(n = 1, 2, \ldots, p + k)$ of the continued fractions $[M/M]_k(x)$. By solving (56) with respect to g_m $(m = 1, 2, \ldots, p)$, we obtain

$$\begin{cases} m = 1, 2, \ldots, p, \quad g_m = c_1^{(m)} \\ \begin{cases} n = 1, 2, \ldots, p - m \\ c_0^{(1+m)} = 1, \quad c_n^{(1+m)} = -\frac{1}{c_1^{(m)}} \left(\sum_{j=0}^{n-1} c_j^{(1+m)} c_{n+1-j}^{(m)} \right) \end{cases} \end{cases} \tag{63}$$

Here $c_m^{(1)}$'s $(m=1,2,\dots,p)$ are the input data, see (2). Equation (59) takes then the following form expressed as a recurrence formula:

$$\begin{cases} n=1,3,\dots,p, \quad C_1^{(n+1)} = g_n / C_1^{(n)} \\ \begin{cases} j=1,2,\dots,k-1 \\ C_{j+1}^{(n+1)} = -\dfrac{\sum_{m=1}^{j} C_{j+2-m}^{(n)} \left(C_m^{(n+1)} + \delta_{2m} \right)}{C_1^{(n)}} - \delta_{2j} \end{cases} \\ C_1^{(n+2)} = g_{n+1} / C_1^{(n+1)} \\ \begin{cases} j=1,2,\dots,k-1 \\ C_{j+1}^{(n+2)} = -\dfrac{\sum_{m=1}^{j} C_{j+2-m}^{(n+1)} \left(C_m^{(n+2)} + \delta_{1m} \right)}{C_1^{(n+1)}} - \delta_{1j} \end{cases} \end{cases} \tag{64}$$

Here g_m $(m=1,2,\dots,p)$ and $C_m^{(1)}$ $(m=1,2,\dots,k)$ are defined by (63) and (4), respectively. The formulae (64) determine the coefficients $C_j^{(p+1)}$ $(j=1,\dots,k)$ in the following recurrence relations:

(i) For an odd p

$$\begin{cases} g_{p+1} = C_1^{(p+1)}, \quad C_j^{(p+1)} = C'^{(1)}_{j-1}, \quad j=2,3,\dots,k \\ m=1,2,\dots,k-1, \quad g_{p+1+m} = C'^{(m)}_1 \\ \begin{cases} n=1,2,\dots,k-1-m \\ C'^{(1+m)}_0 = 1, \quad C'^{(1+m)}_n = -\dfrac{1}{C'^{(m)}_1} \left(\displaystyle\sum_{j=0}^{n-1} C'^{(1+m)}_j C'^{(m)}_{n+1-j} \right) \end{cases} \end{cases} \tag{65}$$

(ii) For an even p

$$\begin{cases} C'^{(1)}_{j+1} = C_j^{(p+1)}, \quad j=1,\dots,k \\ m=1,2,\dots,k, \quad g_{p+m} = C'^{(m)}_1 \\ \begin{cases} n=1,2,\dots,k-m, \\ C'^{(1+m)}_0 = 1, \quad C'^{(1+m)}_n = -\dfrac{1}{C'^{(m)}_1} \left(\displaystyle\sum_{j=0}^{n-1} C'^{(1+m)}_j C'^{(m)}_{n+1-j} \right) \end{cases} \end{cases} \tag{66}$$

Given p terms $c_n^{(1)}$ of the power expansion (2) and k terms $C_n^{(1)}$ of the power series (4), the formulae (63)–(66) provide the coefficients g_n $(n=1,2,\dots p+k)$ for the continued fractions (31). The relations (63)–(66) can also be applied to find the coefficients d_n $(n=1,2,\dots p+k)$ for the continued fractions (32). To this end, one has to replace x by s, p by k and c_n by C_n in (63)–(66).

In the next sections we present some illustrative examples of evaluation of the parameters g_n for continued-fraction representations of two-point Padé approximants $[M/M]_k$, cf. (32).

9. Numerical Test

As an illustration of Theorem 1, the following Stieltjes function is now investigated:

$$xf_1(x) = x\int_1^{1000} \frac{du}{1+xu} = \frac{1}{\ln 1000}\ln\frac{1+1000x}{1+x} \tag{67}$$

According to our general developments, the Stieltjes expansions at $x=0$

$$xf_1(x) = \frac{1}{\ln 1000}\sum_{n=1}^{\infty}\frac{(-1)^n(1-1000^n)}{n}x^n \tag{68}$$

and at $x=\infty$

$$xf_1(x) = 1+\frac{1}{\ln 1000}\sum_{n=2}^{\infty}\frac{(-1)^{n-1}(1-0.001^{n-1})}{n-1}s^{n-1}, \quad s=1/x \tag{69}$$

are the input data for the recurrence relations (63)–(66). The values of g_n ($n = 0,1,2,\ldots,8$) for the continued fractions $[4/4]_k$ ($k = 0,1,\ldots,8$) are displayed in Table 1. Monotone sequences of one-point Padé approximants $[M/M]_0$ constructed from the power series (69) and two-point Padé approximants $[M/M]_k$ corresponding to (68)–(69) are shown in Figs. 1 and 2.

Table 1. Coefficients g_n of the continued fraction $xG^k_{1,s}G^8_{k+1,x}0$ representing two-point Padé approximants $[4/4]_k$ to the Stieltjes function $[\ln((1+1000x)/(1+x))]/\ln 1000$.

	$n=1$	$n=2$	$n=3$	$n=4$	$n=5$	$n=6$	$n=7$	$n=8$
$k=0,\ g_n$	144.6	500.5	166.1	334.3	199.0	301.4	212.7	287.7
$k=1,\ g_n$	1.000	0.007	2.461	233.7	266.8	249.4	251.1	255.5
$k=2,\ g_n$	1.000	0.145	19.91	373.7	215.8	288.9	227.3	275.5
$k=3,\ g_n$	1.000	0.145	0.359	0.018	5.679	253.8	250.9	261.7
$k=4,\ g_n$	1.000	0.145	0.359	0.234	12.07	344.1	227.5	279.9
$k=5,\ g_n$	1.000	0.145	0.359	0.234	0.267	0.022	6.602	262.0
$k=6,\ g_n$	1.000	0.145	0.359	0.234	0.267	0.249	10.29	327.9
$k=7,\ g_n$	1.000	0.145	0.359	0.234	0.267	0.249	0.251	0.024
$k=8,\ g_n$	1.000	0.145	0.359	0.234	0.267	0.249	0.251	0.255

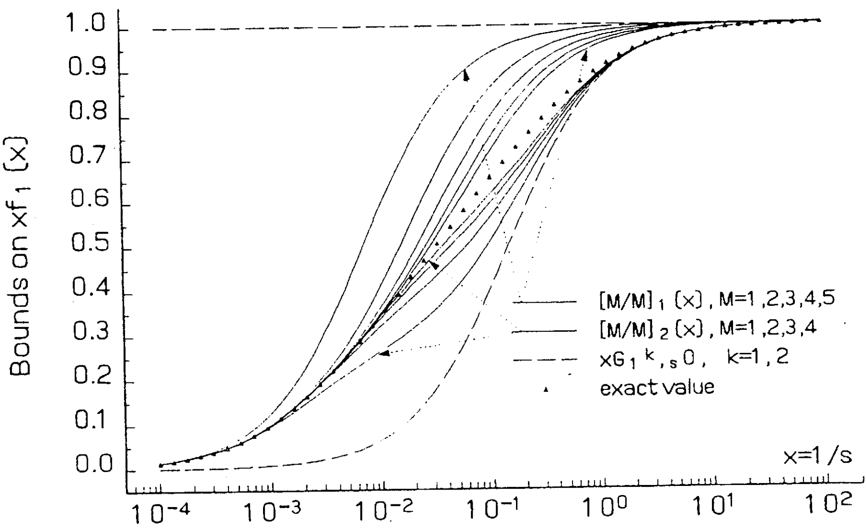

Fig. 1. Sequences of one- ($xG^k_{1,s}0$, $k = 1,2$) and two-point Padé approximants ($[M/M]_k x$), $k = 1, 2$; $M = 1, 2, \ldots, 8$) forming monotone sequences of lower and upper bounds uniformly converging to the Stieltjes function $\ln((1 + 1000x)/(1 + x))/D$, $D = \ln 1000$.

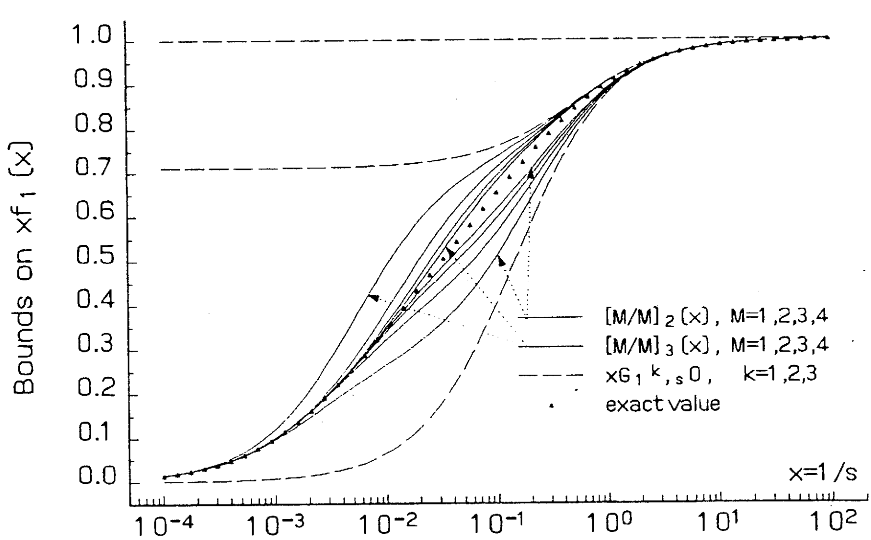

Fig. 2. Sequences of one- ($xG^k_{1,s}0$, $k = 1,2,3$) and two-point Padé approximants ($[M/M]_k(x)$, $k = 1,2$; $M = 1,2,\ldots,8$) forming monotone sequences of lower and upper bounds uniformly converging to the Stieltjes function $\ln((1 + 1000x)/(1 + x))/D$, $D = \ln 1000$.

10. Application to a Physical Problem

To asses the usefulnsess of our results, we are going to study the effective conductivity of an inhomogeneous material which includes regularly-spaced, equally-sized cylinders (Fig. 3). First, let us introduce an appropriate notation: $\Phi = \pi\rho^2$ is the volume fraction, ρ stands for the radius of cylinders, λ_1 and λ_2 are the conductivities of a matrix and inclusions, and $x = (\lambda_2/\lambda_1) - 1$. The bulk conductivity $\lambda_e(x)$ is defined by a linear relationship between the volume-averaged temperature gradient $\langle\overrightarrow{\nabla T}\rangle$ and heat flux $\langle\vec{J}\rangle$:

$$\langle\vec{J}\rangle = \lambda_e(x)\langle\overrightarrow{\nabla T}\rangle \tag{70}$$

The averaging $\langle\cdot\rangle$ is performed over the unit square cell, see Fig. 3. The temperature appearing in (68) satisfies the linear conductivity equation

$$\nabla \cdot \left[(1 + x\theta)\nabla T\right] = 0 \tag{71}$$

where θ is the characteristic function of cylinders. The continuity condition for the normal component of the heat flux $\vec{J} = (1 + x\theta)\overrightarrow{\nabla T}$ at the surfaces of the cylinders is expressed by

$$\vec{m} \cdot \vec{J_-} = \vec{m} \cdot \vec{J_+} \tag{72}$$

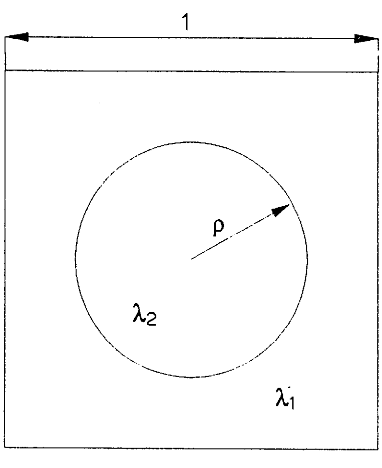

Fig. 3. Unit cell of a square array of equally-sized cylinders.

Here $\vec{m}$ is the unit vector normal to the surface of a cylinder, while $\vec{J_-}$ and $\vec{J_+}$ denote respectively the heat flux on the inside and on the outside of the cylinder surface. It was shown by Bergman (1978) that the effective conductivity $\lambda_e(x)$ determined by (70)–(72) is a Stieltjes function of the type (1).

As the input data for the calculation of $[M/M]_k$ one takes the coefficients of the expansion of $\lambda_e(x)$ at $x = 0$, which have been obtained by Tokarzewski *et al.* (1994a) from the set of equations (70)–(72). Low-order coefficients of the expansion of $\lambda_e(s)$ at

$s = 0$, where $s = 1/x$, are reported by McPhedran *et al.* (1988). Starting from these two truncated series, the sequences of two-point Padé approximants $[M/M]_k$ ($k = 0, 1, 2$; $M = 1, 2, \dots, 18$) to the effective conductivity $\lambda_e(x)$ were calculated via (63)–(66). The numerical results are presented by Tokarzewski *et al.* (1994a).

Let us concentrate on the two-point Padé approximant $[2/2]_2$ corresponding to

$$\lambda_e(x)/\lambda_1 - 1 = c_1^{(1)} x + c_2^{(1)} x^2 + o(x^2), \quad c_1^{(1)} = \Phi, \quad c_2^{(1)} = 1 - \Phi \tag{73}$$

and

$$\lambda_e(x)/\lambda_1 - 1 = C_1^{(1)} + C_2^{(1)} s^1 + o(s^1), \quad C_1^{(1)} = \pi(d-1) - 1 \tag{74}$$

with $C_2^{(1)} = -2\pi d(d-1)\ln(d)$, $d = \sqrt{\pi/(\pi - 4\phi)}$, $\phi = \pi\rho^2$, $s = 1/x$. The truncated series (73) and (74) are given by Bergman (1978) and McPhedran *et al.* (1988), respectively. By using (63)–(66) and (32) we obtain

$$[2/2]_2(x) = G_{1,x}^2 G_{3,s}^4 0 = \frac{H_1 x(1 + H_4 x)}{(1 + H_4 x)(1 + H_2 x) + H_3 x} \tag{75}$$

where

$$H_1 = c_1^{(1)}, \quad H_2 = \frac{c_1^{(1)}}{C_1^{(1)}}, \quad H_3 = -\frac{c_2^{(1)}}{c_1^{(1)}} - \frac{c_1^{(1)}}{C_1^{(1)}}, \quad H_4 = \frac{C_2^{(1)}}{c_1^{(1)}} \frac{C_1^{(1)} c_2^{(1)} + (c_1^{(1)})^2}{c_1^{(1)} C_2^{(1)} + (C_1^{(1)})^2} \tag{76}$$

The numerical values of the function (74) are shown in Fig. 4. For comparison, the asymptotic solution proposed by McPhedran *et al.* (1988) and upper bounds $[M/M]_1$ reported by Tokarzewski *et al.* (1994a), are also depicted. From Fig. 4, it follows that the accuracy of the simple formula

$$\lambda_e(x)/\lambda_1 = 1 + [2/2]_2 \tag{77}$$

is acceptable for a wide range of the parameters Φ and x.

11. Concluding Remarks

By using special continued fractions representing two-point Padé approximants it has been proved that: (i) Carleman's criterion derived for one-point Padé approximants applies also to two-point Padé ones, (ii) under some assumptions the balanced and unbalanced two-point Padé approximants form in a real domain monotone sequences of lower and upper bounds converging to a Stieltjes function, (iii) the fundamental inequalities for one-point Padé approximants given by (17) have been extended to the case of two-point Padé ones, cf. (46) and (47).

The main theoretical result of this paper given by Theorem 1 solves the problem of the monotone and uniform convergence of both the balanced and unbalanced two-point Padé approximants to a Stieltjes function $xf_1(x)$ represented by the asymptotic expansions of $xf_1(x)$ at $x = 0$ and $x = \infty$.

The general recurrence formulae (63)–(66) for finding two-point Padé approximants from the asymptotic expansions (2) and (4) has been derived and tested successfully for correctness (Figs. 1 and 2).

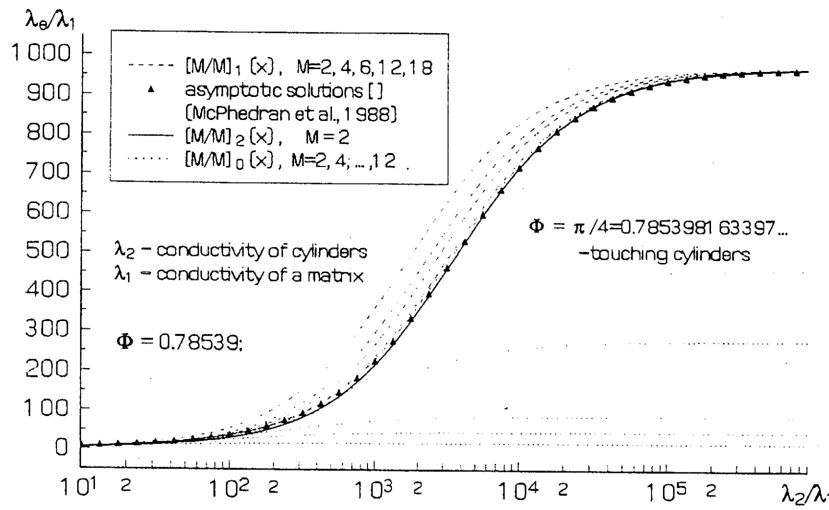

Fig. 4. One- and two-point Padé approximants to the effective conductivity $\lambda_e(x)/\lambda_1$ of a square array of cylinders for $\Phi = 0.78539$.

As an example of a practical application, the effective conductivity of a square array of equally-sized, highly-conducting cylinders has been investigated in terms of two-point Padé approximant bounds on $\lambda_e(x)/\lambda_1$, cf. Fig. 4.

Theorem 1 also applies to the analysis of mathematically similar quantities, e.g. the overall electrical or magnetical conductivities, dielectric constants and many others.

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