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TWO-POINT PADE APPROXIMANTS FOR STIELTJES SERIES

Abstract

We have proved that certain two-point Pade approximants to Stieltjes series occupying the diagonal of the Pade table form sequences of lower and upper bounds uniformly converging to Stieltjes function. The results can be applied in the theory of inhomogeneous media to calculate the bounds on the effective transport coefficients of heterogeneous materials.

1. Introduction.

The mathematical properties of one-point Pade approximants to Stieltjes functions have been extensively investigated in recent years [1-6]. One of the most important results presented in literature [1-6] states , that the sequence of one-point Pade approximants represented by the convergents of a continued fraction of type S [1-6] form upper and lower bounds uniformly approaching the Stieltjes function. Moreover these bounds are the best in respect to the given numbers of power series coefficients.

On the contrary the mathematical properties of the two-point Pade approximants generated by two different power expansions of Stieltjes function have not been examined in detail. In particular the problem of uniform convergence of two-point Pade approximants to the Stieltjes function has not been investigated.

In this paper the two types of two-point Pade approximants occupying diagonal of the Pade table will be theoretically examined. The first type matches at infinity the value of the Stieltjes function, whereas the second type fits at infinity both the value and the first derivative of the Stieltjes function.

The main aim of this paper is to prove that the two-point Pade approximants investigated in this paper form sequences of upper and lower bounds uniformly approaching the Stieltjes function. The obtained bounds are the best in respect to the given numbers of Stieltjes series coefficients. Moreover the convergence of the two point Pade approximants is more rapid then the convergence of one-point Pade approximants investigated in literature [1-6].

As an example of practical applications the bounds on the effective conductivity of square array of cylinders has been calculated for the range of parameters, for which the numerical methods used in the theory of dispersed media fail [7].

2. Basic definitions.

The starting point for our considerations is a Stieltjes function f(z) defined in the interval $0 \le z \le \infty$ by means of the following Stieltjes-integral representation

$$f(z) = z \int_0^\infty \frac{\Phi(u)}{1+zu}\, du, \tag{2.1}$$

where spectral density $\Phi(u)$ is assumed to be real and positive. The power series expansion of Stieltjes function (2.1) at z=0

$$f(z) = \sum_{n=1}^{\infty} c_n (-z)^n, \tag{2.2}$$

where

$$c_n = \int_0^\infty u^{n-1}\ \Phi(u)\ du, \qquad n=1,2,.. \tag{2.3}$$

and at $z = \infty$

$$f(z) = \sum_{n=0}^{\infty} c_{-n}(-z)^{-n}, \tag{2.4}$$

where

$$c_n = \int_0^\infty u^{-n-1}\ \Phi(u)\ du, \qquad n=1,2, \tag{2.5}$$

will be also considering. The coefficients c_n (2.3), (2.5) are assumed to take only finite values. The power expansions (2.2), (2.4) with constraints (2.3) and (2.5) are called the Stieltjes series [1-6]. The sequence of two-point Pade approximants calculated for series (2.2), (2.4) take the following general form

$$[M/M]_k = \frac{L_{k,M}(z)}{Q_{k,M}(z)} = \frac{a_{1,k}\ z + a_{2,k}\ z^2 + \cdots\ a_{M,k}\ z^M}{1 + b_{1,k}\ z + b_{2,k}\ z^2 + \cdots\ b_{M,k}\ z^M}. \tag{2.6}$$

It will be needed for further considerations the power series expansion of the function (2.6) at zero

$$[M/M]_k = \sum_{n=1}^{\infty} c_{n,k}(-z)^n; \tag{2.7}$$

and at infinity

$$[M/M]_k = \sum_{n=0}^{\infty} c_{-n,k}(-z)^{-n}. \tag{2.8}$$

Now we are ready to explain the notation $[M/M]_k$ determining the two-point Pade approximants (2.6). If 2M-k coefficients $c_{n,k}$ of the series (2.7) and k coefficients $c_{-n,k}$ of the series (2.8) are matching the first 2M-k coefficients c_n of (2.2) and k coefficients c_{-n} of (2.4) the two-point Pade approximants to Stieltjes function (2.1) will be denoted by $[M/M]_k$ (2.6). It easy to notice, that according to the above notation $[M/M]_0$ denotes the one-point Pade approximants. Two-point Pade approximants (2.6) can be expressed also in alternative way as a S continued fractions [1] depending on z

$$[M/M]_k = \frac{g_{1,k}\ z}{1} + \cdot\cdot \frac{g_{2M-k,k}\ z}{1} + \cdot\cdot\cdot \frac{G_{2M-k+1,k}\ z}{1} + \cdot\cdot \frac{G_{2M,k}\ z}{1} \tag{2.9}$$

and on s

$$[M/M]_k = \frac{g_{1,k}}{s +} \frac{g_{2,k}}{1} + \cdot\cdot \frac{g_{2M-k,k}}{s} + \cdot\cdot \frac{G_{2M-k+1,k}}{s} + \cdot \frac{G_{2M,k}}{1}, \tag{2.10}$$

where

$$s = 1/z. \tag{2.11}$$

The coefficients $g_{1,k}$, ... ,$g_{2M-k,k}$ of a continued fractions (2.9) and (2.10) are uniquely determined by the 2M-k coefficients c_n, n=1,2, .. ,2M-k of a Stieltjes series (2.2). To calculate the remaining coefficients $G_{2M-k+1,k}$, .. ,$G_{2M,k}$ the values of k coefficients of a series (2.4) c_{-n}, n=1,2,..,k are additionally needed.

3. One-point Pade approximants $[M/M]_0$

Substituting k=0 into expression (2.10) we obtain the one-point Pade approximants $[M/M]_o$ in the form of S continued fractions [1-6]

$$[M/M]_o = \frac{g_{1,0}}{s} + \frac{g_{2,0}}{1} + \cdot\cdot \frac{g_{2M-1,0}}{s} + \frac{g_{2M,0}}{1}. \tag{3.1}$$

On the contrary to the two-point Pade approximants $[M/M]_k$,k=1,2,..the one-point Pade approximants $[M/M]_k$,k= 0 constructed for Stieltjes series has been extensively investigated [1-6]. The main, theoretical results presented in literature, which are needed for our investigations are as follows: 1) the coefficients of a continued fraction $[M/M]_o$ (3.1) takes only positive values

$$g_{n,0} \geq 0; \qquad (3.2)$$

2) the following inequality holds for any positive value of $g_{2M,0}$

$$\frac{\partial}{\partial g_{2M,0}}[M/M]_0 < 0; \qquad (3.3)$$

3) sequence of one-point Pade approximants $[M/M]_o$ constructed for the Stieltjes series (2.2) forms upper and lower bounds on the function f(z) (2.1).

$$[M/M\text{-}1]_0 \geq [M+1/M]_0 \geq f(z) \geq [M+1/M+1]_0 \geq [M/M]_0, \qquad (3.4)$$

4)the bounds get better if M increases :

$$\lim_{M\to\infty} \{[M+1/M]_0 = [M/M]_0\} = f(z). \qquad (3.5)$$

It follows from relations (3.4) and (3.5) that a sequence of a one-point Pade approximants uniformly converges to the function f(z) (2.1). The inequality (3.4) and the equality (3.5) has been proved only for case of one-point Pade approximants $[M/M]_k$, k=0 [1-4]. The main task of this paper is to extend the validity of relations (3.4) and (3.5) respectively on the case of two-point Pade approximants $[M/M]_k$, k=1 and $[M/M]_k$, k=2.

4. Convergence of two-point Pade approximants $[M/M]_1$

Substituting into (2.10) k=1 we obtain two-point Pade approximants $[M/M]_1$ as follows

$$[M/M]_1 = \frac{g_{1,1}}{s} + \frac{g_{2,1}}{1} + \cdots \frac{g_{2M-1,1}}{s} + \frac{G_{2M,1}}{1}. \qquad (4.1)$$

It necessary to notice that coefficients of continued fractions (3.1) and (4.1) are equal to each other up to 2M-1 term, because they are both calculated on the base of 2M-1 power series coefficients (2.2).

$$g_{n,0} = g_{n,1}\,, \qquad n=1,2,..2M-1. \qquad (4.2)$$

The last coefficient of (4.1) $G_{2M,1}$ is determined by the equation

$$\left\{ \frac{g_{1,0}}{s} + \frac{g_{2,1}}{1} + \cdots \frac{g_{2M-1,0}}{s} + \cdots \frac{G_{2M,1}}{1} \right\}_{s=0} = c_0, \tag{4.3}$$

where c_0 denotes the first term of a series (2.4). On the base on the inequality (3.4) we can write

$$\left\{[M/M-1]_0\right\}_{s=0} \geq c_0 \geq \left\{[M/M]_0\right\}_{s=0} \tag{4.4}$$

It is convenient to write the inequality (4.4) by means of the continued fractions of type S

$$\left\{ \frac{g_{1,0}}{s} + \cdots \frac{g_{2M-1,0}}{s} + \frac{0}{1} \right\}_{s=0} \geq c_0 > \left\{ \frac{g_{1,0}}{s} + \cdots \frac{g_{2M,0}}{1} \right\}_{s=0} , \tag{4.5}$$

where in the left hand side of relation (4.5) the vanishing term 0/1 is introduced explicitly for easier analysis. Substituting (4.3) into (4.5) and comparing appropriate terms in all continued fractions (4.3), (4.5) we come, due to (3.3), to the following important conclusion

$$0 \leq G_{2M,1} \leq g_{2M,0}. \tag{4.6}$$

It follows from (3.2), (4.2) and (4.6) that the denominator $Q_{1,M}(z)$ of the two-point Pade approximant $[M/M]_1$ (2.6), (4.1) takes positive values

$$Q_{1,M}(z) \geq 0. \tag{4.7}$$

Owing to (4.6) the validity of relation (4.5) can be extended on all positive values of s. Hence we can write

$$[M/M-1]_0 \geq [M/M]_1 \geq [M/M]_0. \tag{4.8}$$

The sequence of one-point Pade approximants $[M/M]_0$ and $[M/M-1]_0$ is convergent to the function f(z) (2.1). Hence we can write immediately

$$\lim_{M\to\infty} [M/M]_1 = f(z). \tag{4.9}$$

Both the sequence of one-point Pade approximants $[M/M]_0$ calculated for the Stieltjes series (2.2) and the sequence of two-point Pade approximants $[M/M]_1$ constructed for series (2.2) and (2.4) are convergent to the function f(z) (2.1)

5. Inequalities for Pade approximants $[M/M]_1$

The following relation expressing the difference of the two successive approximants $[M/M]_1$

$$[M+1/M+1]_1-[M/M]_1 = \frac{W_1(M+1/M)\ z^{2M}}{Q_{1,M}(z)\cdot Q_{1,M+1}(z)} \tag{5.1}$$

is a consequence of the definition of two-point Pade approximants (2.6). Dividing both sides of (5.1) by z^{2M} we obtain for $z = 0$

$$c_{2M}-c_{2M,1} = W_1(M+1/M), \tag{5.2}$$

where c_{2M} and $c_{2M,1}$ are respectively, the 2M-th coefficient of the power series (2.2), the 2M-th coefficient of the power series (2.7). On the base of the definition of Pade approximants (2.6) the following equality holds

$$\frac{\partial^{2M}}{\partial z^{2M}}\left\{[M/M]_0-[M/M]_1\right\}_{z=0} = (2M)!\ [c_{2M}-c_{2M,1}]. \tag{5.3}$$

From (5.2) and (5.3) follows

$$W_1(M+1/M) = \frac{1}{(2M)!}\ \frac{\partial^{2M}}{\partial z^{2M}}\left\{[M/M]_0-[M/M]_1\right\}_{z=0}. \tag{5.4}$$

Due to (4.6) we can write

$$[M/M]_0-[M/M]_1 \le 0. \tag{5.5}$$

The first term of power series expansion of the left side of inequality (5.5) is equal, on the base on (5.4) and definition of two-points Pade approximants (2.6), to $W_1(M+1/M)\ z^{2M}$. Hence from (5.5) follows

$$W_1(M+1/M) \le 0. \tag{5.6}$$

The denominators $Q_{1,M}(z)$ and $Q_{1,M+1}(z)$ take positive values (4.7). Therefore from (5.1) and (5.6) we have

$$[M+1/M+1]_1 - [M/M]_1 \leq 0 \tag{5.7}$$

and due to (4.9)

$$[M/M]_1 \geq [M+1/M+1]_1 \geq f(z). \tag{5.8}$$

The two-point Pade approximants $[M/M]_1$ form the sequence of upper bounds uniformly converging to the function f(z) (2.1). The bounds get better, when M increases.

6.Convergence of two-point Pade approximants $[M/M]_2$

Substituting into (2.10) k=2 we obtain

$$[M/M]_2 = \frac{g_{1,2}}{s +} \frac{g_{2,2}}{1} + \cdots \frac{g_{2M-2,2}}{s} + \cdots \frac{G_{2M-1,2}}{s} + \frac{\rho\, G_{2M-1,2}}{1}. \tag{6.1}$$

where for convenience of further investigations we substituted

$$G_{2M,2} = \rho\, G_{2M-1,2} \tag{6.2}$$

The continued fractions $[M/M]_1$ (4.1) and $[M/M]_2$ (6.1) have a 2M-2 equal coefficients

$$g_{n,1} = g_{n,2}\ , \qquad n=1,2,\dots,2M-2 \tag{6.3}$$

determined by 2M-2 power series coefficients (2.2). The remaining coefficients ρ and $G_{2M-1,2}$ are determined by the following two equations

$$\left\{[M/M]_2\right\}_{s=0} = c_0\ , \quad \frac{\partial}{\partial s}\left\{[M/M]_2\right\}_{s=0} = -c_1, \tag{6.4}$$

where c_0 and $-c_1$ are the power series coefficients (2.4). Analyzing the relations (4.1), (6.1), (6.3) and (6.4) we get

$$\rho = \frac{G_{2M,1}}{g_{2M-1,1}} > 0. \tag{6.5}$$

Due to the equalities (6.5) the continued fraction (4.1) can be written as follows

$$[M/M]_1 = \frac{g_{1,1}}{s} + \frac{g_{2,1}}{1} + \cdots \frac{g_{2M-1,1}}{s} + \frac{\rho \cdot g_{2M-1,1}}{1}. \tag{6.6}$$

The coefficients $g_{1,1},\dots,g_{2M-1,1}$ are positive (3.2), (4.2). Then for $[M/M]_1$ expressed by (6.6) the following relations

$$\frac{\partial}{\partial g_{2M-1,1}} [M/M]_1 > 0 , \quad \text{for } g_{2M,1} > 0 \tag{6.7}$$

and

$$\left\{[M/M]_1\right\}_{s=0} = c_0, \quad \text{for } g_{2M-1,1} > 0 \tag{6.8}$$

are satisfied. On the base on (6.7) and (6.8) we have at once

$$\frac{\partial}{\partial g_{2M-1,1}} \left\{\frac{\partial}{\partial s} [M/M]_1\right\}_{s=0} > 0, \quad \text{for } g_{2M-1,1} > 0. \tag{6.9}$$

For $[M/M]_1$ expressed by (6.6) the first derivative in respect to s increases at s=0, when coefficient $g_{2M-1,1}$ grows up. It is convenient to introduce a positive number ε

$$0 \le \varepsilon \ll 1 \tag{6.10}$$

chosen so small, that the following relation is satisfied

$$\frac{\partial}{\partial s} \left\{ \frac{g_{1,1}}{s} + \frac{g_{2,1}}{1} + \cdots \frac{\varepsilon}{s} + \frac{\rho \cdot \varepsilon}{1} \right\}_{s=0} \le -c_1. \tag{6.11}$$

It necessary to notice that due to (6.8) (6.9) and (3.4) the left hand side of inequality (6.11) tends to minus infinity when ε approaching zero. On the base on (5.8) and (6.8) we have

$$-c_1 \le \frac{\partial}{\partial s} \left\{ \frac{g_{1,1}}{s} + \frac{g_{2,1}}{1} + \cdots \frac{g_{2M-1,1}}{s} + \frac{\rho \cdot g_{2M-1,1}}{1} \right\}_{s=0}. \tag{6.12}$$

The coefficient $-c_1$ is equal to

$$-c_1 = \frac{\partial}{\partial s}\left\{ \frac{g_{1,1}}{s} + \frac{g_{2,1}}{1} + \cdots \frac{G_{2M-1,2}}{s} + \frac{\rho \cdot G_{2M-1,2}}{1} \right\}_{s=0} . \qquad (6.13)$$

Analyzing (6.11-6.13) and (6.9) we come to the following conclusion

$$0 \le \varepsilon \le G_{2M-1,2} \le g_{2M-1,1}. \qquad (6.14)$$

From (6.1), (6.4) and (6.14) follows important inequality

$$Q_{2,M}(z) > 0, \qquad (6.15)$$

where $Q_{2,M}(z)$ (2.6) denotes the denominator of the two-point Pade approximant $[M/M]_2$ (6.1). Additionally due to relations (6.14) and inequalities (3.4) we have

$$[M\text{-}2/M\text{-}2]_0 \le [M/M]_2 \le [M/M]_1. \qquad (6.16)$$

The approximants $[M\text{-}2/M\text{-}2]_0$ and $[M/M]_1$ are convergent to the function f(z) (2.1) . Hence we obtain

$$\lim_{M\to\infty} = [M/M]_2 = f(z). \qquad (6.17)$$

Both the sequence of one-point Pade approximants $[M/M]_0$ constructed for the Stieltjes series (2.2) and the sequence of two-point Pade approximants $[M/M]_2$ calculated for (2.2-2.4) are convergent to the function f(z) (2.1).

7. Inequalities for two-point Pade approximants $[M/M]_2$

The following relation expresses the difference of the two successive approximants of a type $[M/M]_2$

$$[M+1/M+1]_2 - [M/M]_2 = \frac{W_2(M+1/M)\ z^{2M-1}}{Q_{2,M}(z)\cdot Q_{2,M+1}(z)}. \qquad (7.1)$$

The form of a right hand side of the equation (7.1) is a consequence of the definition of the two-point Pade approximants (2.6). Following the argumentation presented in paragraph 5 we can write relation

$$W_2(M+1/M) = \frac{\partial^{2M-1}}{\partial z^{2M-1}} \left\{[M/M]_1-[M/M]_2\right\}_{z=0} \tag{7.2}$$

similar to expression (5.4). Moreover due to (6.14) the following inequality holds

$$[M/M]_1-[M/M]_2 \geq 0. \tag{7.3}$$

On the base on (7.2) and (7.3) we have at once

$$W_2(M+1/M) \geq 0. \tag{7.4}$$

The relations (6.15) , (7.4) (7.1) lead to the following important inequality

$$[M+1/M+1]_2-[M/M]_2 \geq 0. \tag{7.5}$$

Hence on the base on (6.17) and (7.5) we have

$$f(z) \leq [M+1/M+1]_2 \leq [M/M]_2. \tag{7.6}$$

The two-point Pade approximants $[M/M]_2$ form the sequence of lower bounds converging to the Stieltjes function f(z) (2.1). The bounds get better, when M increases.

8. Numerical example

To illustrate the inequalities (5.8), (7.6) and (3.4) we introduce the spectral density

$$\Phi(u) = \begin{cases} 0 & 0 \leq u \leq 1 \\ 1 & 1 < u < 1000 \\ 0 & 1000 \leq u \leq \infty \end{cases} \tag{8.1}$$

leading to the following Stieltjes function

$$f(z) = z \int_1^{1000} \frac{1}{1+zu}\, du = \ln\frac{1+1000z}{1+z}. \tag{8.2}$$

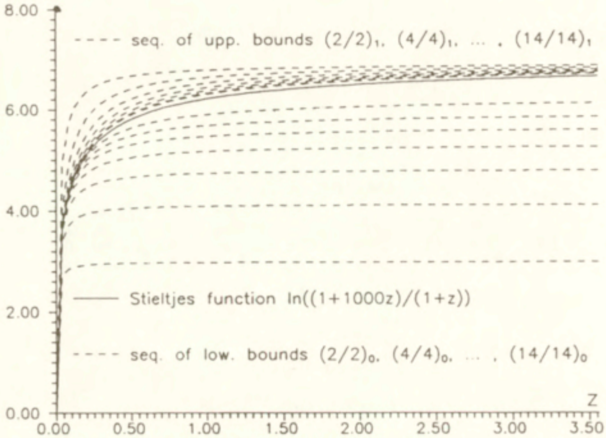

Fig.1 The sequence of two-point Pade approximants of type 0 and 1 forming upper and lower bounds for Stieltjes function

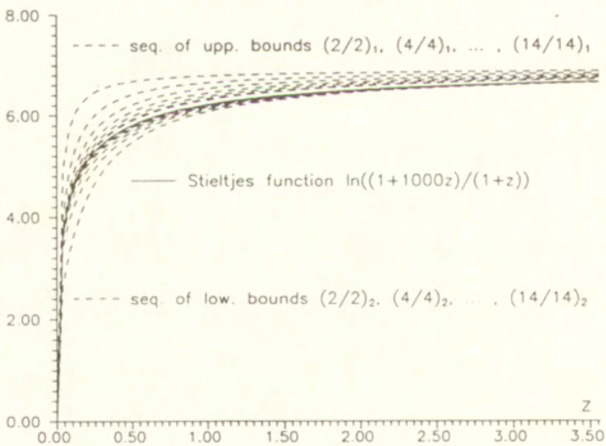

Fig.2 The sequence of two-point Pade approximants of type 1 and 2 forming upper and lower bounds for the Stieltjes function

The two Stieltjes power series expanded at zero

$$f(z) = \sum_{n=1}^{\infty} \frac{1}{n} (1-1000^n)(-z)^n \qquad (8.3)$$

and at infinity

$$f(z) = \ln(1000) + \sum_{n=1}^{\infty} \frac{1}{n} (1-0.001^n)(-z)^{-n} \qquad (8.4)$$

result immediately from (8.2). Using algorithm FG [5] the sequences of two-point Pade approximants of type $[M/M]_1$

$$[2/2]_1 \ , \ [4/4]_1 \ ,\ldots, \ [14/14]_1, \qquad (8.5)$$

of type $[M/M]_2$

$$[2/2]_2 \ , \ [4/4]_2 \ ,\ldots, \ [14/14]_2, \qquad (8.6)$$

and of type $[M/M]_0$

$$[2/2]_0 \ , \ [4/4]_0 \ ,\ldots, \ [14/14]_0 \qquad (8.7)$$

has been calculated. Numerical results drawn in figure 1 and 2 illustrate uniform convergence of two-point Pade approximants to the Stieltjes function.

9. Application to the theory of dispersed media.

It has been proved in the theory of dispersed media [8] that effective transport coefficients of two-phase composites represented by an eigenvalues of a second order tensor have Stieltjes-integral representations (2.1) [8]. Hence all theoretical results presented in this paper can be applied in the theory of dispersed media to determine the effective properties of two-phase composites. As an example, a heterogeneous material consisting of equal- sized cylinders arrange in a square array, has been investigated [7]. For a wide range of parameters the upper and lower bounds on the effective conductivity coefficient has been obtained in the form of two-point Pade approximants $[M/M]_1$ and $[M/M]_2$. The bounds presented in paper [7] are much better then the one-point Pade approximants bounds reported in literature [9].

10. Final remarks

Using continued fraction representation it has been proved that two-point Pade approximants $[M/M]_1$ and $[M/M]_2$ form respectively upper and lower bounds uniformly converging to the Stieltjes function. Numerical experiments suggest that the two-point Pade approximants $[M/M]_3$ and $[M/M]_4$, $[M/M]_5$ and $[M/M]_6$ and so on also form sequences of upper and lower bounds uniformly approaching the Stieltjes function. These numerical observations will be examined theoretically in the next paper.

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