К О Р О Т К І   П О В І Д О М Л Е Н Н Я

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APPROXIMATION OF SMOOTH FUNCTIONS BY WEIGHTED MEANS OF N-POINT PADÉ APPROXIMANTS

НАБЛИЖЕННЯ ГЛАДКИХ ФУНКЦІЙ ЗВАЖЕНИМИ СЕРЕДНІМИ N-ТОЧКОВИХ АПРОКСИМАНТ ПАДЕ

Let f be a function we wish to approximate on the interval $[x_1, x_N]$ knowing $p_1 > 1, p_2, \ldots, p_N$ coefficients of expansion of f at the points $x_1, x_2, \ldots, x_N$. We start by computing two neighboring N-point Padé approximants (NPAs) of f, namely $f_1 = [m/n]$ and $f_2 = [m-1/n]$ of f. The second NPA is computed with the reduced amount of information by removing the last coefficient from the expansion of f at x_1. We assume that f is sufficiently smooth, (e.g. convex-like function), and (this is essential) that f_1 and f_2 bound f in each interval $]x_i, x_{i+1}[$ on the opposite sides (we call the existence of such two-sided approximants the TSE property of f). Whether this is the case for a given function f is not necessarily known a priori, however, as illustrated by examples below it holds for many functions of practical interest. In such case further steps become relatively simple. We select a known function s having the TSE property with values $s(x_i)$ as close as possible to the values $f(x_i)$. We than compute the approximants $s_1 = [m/n]$ and $s_2 = [m-1/n]$ using the values at points x_i and determine for all x the weight function α from the equation $s = \alpha s_1 + (1-\alpha)s_2$. Applying this weight to calculate the weighted mean $\alpha f_1 + (1-\alpha) f_2$ we obtain significantly improved approximation of f.

Розглянемо функцію, яку ми хочемо апроксимувати на інтервалі $[x_1, x_N]$, якщо відомі $p_1 > 1, p_2, \ldots, p_N$ коефіцієнтів розкладу f у точках $x_1, x_2, \ldots, x_N$. Спочатку ми знаходимо дві сусідні N-точкові апроксиманти Паде (НАП) функції f, а саме $f_1 = [m/n]$ та $f_2 = [m-1/n]$ для f. Другу НАП знаходимо за обмеженою кількістю інформації шляхом видалення останнього коефіцієнта розкладу f у точці x_1. Припустимо, що f — достатньо гладка функція (наприклад, опуклого типу) та (це суттєво) f_1 і f_2 обмежують f у кожному інтервалі $]x_i, x_{i+1}[$ з протилежних сторін (умову існування таких двосторонніх апроксимант ми називаємо TSE властивістю f). A priori необов'язково відомо, що це припущення виконується для заданої функції f. Водночас, як показано на прикладах, що наведені нижче, воно виконується для багатьох функцій, цікавих з практичної точки зору. В такому випадку подальші кроки стають відносно простими. Виберемо відому функцію s з TSE властивістю та значеннями $s(x_i)$ настільки близькими до значень $f(x_i)$, наскільки це можливо. Далі ми знаходимо апроксиманти $s_1 = [m/n]$ та $s_2 = [m-1/n]$ за значеннями в точках x_i і визначаємо для будь-якого x вагову функцію α з рівняння $s = \alpha s_1 + (1-\alpha)s_2$. Застосовуючи цю вагу при знаходженні зваженого середнього $\alpha f_1 + (1-\alpha) f_2$, отримуємо значно покращене наближення f.

1. Introduction. In this section we briefly summarize the essential properties of the NPAs and the role played by the TSE property in what amounts to a magic wand in the proposed method. In Section 2 we analyze certain technical problems related to the rescaling of the reference function and some simplifications in calculating weights used in determining the weighted mean approximations. In the remaining sections we illustrate application of the proposed method to some functions of interest.

1.1. Neighboring N-point Padé approximants. Let f be an analytic function at N different real points

$$-R < x_1 < x_2 < \ldots < x_N < \infty \qquad (1)$$

having the power expansions

$$\sum_{k=0}^{p_j - 1} c_k(x_j)(x - x_j)^k + O\Big((x - x_j)^{p_j}\Big), \quad j = 1, \ldots, N, \qquad (2)$$

then the N-point Padé approximant to f, if it exists, is a rational function P_m/Q_n noted as follows:

$$[m/n]^{p_1 p_2 \ldots p_N}_{x_1 x_2 \ldots x_N}(x) = \frac{a_0 + a_1 x + \ldots + a_m x^m}{1 + b_1 x + \ldots + b_n x^n}, \qquad m + n + 1 = p = p_1 + p_2 + \ldots + p_N, \quad (3)$$

and satisfying the following relations:

$$f(x) - [m/n](x) = O\Big((x - x_j)^{p_j}\Big), \quad j = 1, 2, \ldots, N, \quad (4)$$

where each p_j represents the number of coefficients $c_k(x_j)$ of expansion (2) actually used for the computation of NPA given by (3).

In the following we always label the NPA computed with all available values using index "1", as $f_1 = [m/n]$, and the NPA computed using the number of values reduced by one with index "2", as $f_2 = [m-1/n]$. In all cases, we remove the last coefficient from the expansion of f or s at x_1 when calculating f_2 or s_2.

1.2. Two-sided estimates property (TSE property). The proposed method of approximation is based largely on the TSE property which was first proved for the Stieltjes functions by Michael Barnsley [1]. Let us introduce (see [4, 5]) a nondecreasing step-wise function L

$$L(x) = \sum_{j=1}^{N} p_j H(x - x_j),$$

where H is a Heaviside function. $L(x)$ represents the total number of coefficients in power series expansions of f at all points $x_j \leq x$:

$$L(x_k) = p_1 + p_2 + \ldots + p_k, \qquad L(x_N) = p = \sum_{j=1}^{N} p_j.$$

Theorem 1. *Let s be a Stieltjes function, then the diagonal $s_1 = [k/k]$ and subdiagonal $s_2 =$ $= [k-1/k]$ N-point Padé approximants to s satisfy the following inequality*:

$$(-1)^{L(x)}[m/n](x) \leq (-1)^{L(x)} s(x), \quad x \in]-R, \infty[. \quad (5)$$

After removing one coefficient at x_1, s_2 becomes exactly $[k-1/k]^{p_1 - 1 \ldots p_N}_{x_1 \ldots x_N}$.

Similar theorem for particular non-Stieltjes functions was proven in [4].

Theorem 2. *Let $s(x) = s(x_1) + (x - x_1)h(x)$, where h is a Stieltjes function, then the subdiagonal $s_1 = [k+1/k]$ and diagonal $s_2 = [k/k]$ N-point Padé approximants to s satisfy the following inequality*:

$$(-1)^{L(x)}[m/n](x) \geq (-1)^{L(x)} s(x), \quad x \in]-R, \infty[. \quad (6)$$

Above theorems prove the TSE property for Stieltjes and Stieltjes-like functions, however this property also holds for a wider class of functions, as illustrated below. For $x < x_1$ all NPAs are smaller than s. Starting from x_1, s_2 bounds s on the opposite side with respect to s_1 in each interval $[x_i, x_{i+1}]$. The convergence of NPAs to the Stieltjes functions being very rapid, s_1 is a considerably better approximation of s in $[x_1, x_N]$ than s_2: $|s - s_1| \ll |s - s_2|$. In fact this is observed also for the non-Stieltjes functions. We can further improve the approximation f_1 of f by finding the weighted means m_i in each interval $[x_i, x_{i+1}]$ such that

$$\forall x \in [x_i, x_{i+1}]\colon \quad |f - m_i| < |f - f_1|, \quad i = 1, 2, \ldots, N-1. \quad (7)$$

1.3. Finding a suitable reference function. Suppose we wish to approximate some smooth function f on the interval $[x_1, x_N]$ knowing $p_1 > 1,\ p_2, \ldots, p_N$ coefficients of expansion of f at the points $x_1, x_2, \ldots, x_N$. Additionally, let the values $f(x_i)$ be regularly distributed, as in the case of monotonic interpolations of Stieltjes functions at real arguments. We proceed as follows: first we select similar known function having the TSE property. Next we rescale this function to obtain the reference function s which should be close to f. For instance we can require that

$$s(x_1) = f(x_1) \qquad \text{and} \qquad s(x_N) = f(x_N). \tag{8}$$

Since we know the analytic form of the reference function s, we can compute for each x the exact weight function α from the following equation:

$$s(x) = \alpha(x)s_1(x) + (1 - \alpha(x))s_2(x) \qquad \text{that is:} \qquad \alpha(x) = \frac{s(x) - s_2(x)}{s_1(x) - s_2(x)}. \tag{9}$$

Now we compute two NPAs f_1 and f_2 of f, expecting that they are located on the opposite sides of f in each subinterval. We also compute similar NPAs s_1 and s_2 of s and then using (9), we calculate the weight function α. The basic idea of our method boils down to the use of weight function α determined for the reference function s to compute the weighted mean of approximants f_1 and f_2. This is the *magic wand* which delivers the improved approximation.

To simplify the calculations we define in each interval the weights and the weighted means as follows:

$$\begin{gathered} \alpha_i = \alpha\Big(\frac{x_i + x_{i+1}}{2}\Big), \quad i = 1, 2, \ldots, N-1, \\ m_i(x) = \alpha_i f_1(x) + (1 - \alpha_i) f_2(x), \quad x \in [x_i, x_{i+1}], \end{gathered} \tag{10}$$

expecting that they will give a good approximation of f. This approximation has the following properties due to the condition (8) of rescaling:

$$m_1(x_1) = f(x_1) = f_1(x_1) = f_2(x_1) = s(x_1) = s_1(x_1) = s_2(x_1),$$

$$m_{N-1}(x_N) = f(x_N) = f_1(x_N) = f_2(x_N) = s(x_N) = s_1(x_N) = s_2(x_N).$$

2. General method of approximation and the problem of rescaling. The Introduction presents the basic ideas of the presented method of approximation. Practical application of the proposed method requires some additional considerations.

Reference function. Two properties are required for the reference function s. One is the TSE property, i.e., the existence of the two sided estimates. This is the case for many real functions such as Stieltjes functions, function $(a + bx)h(x)$, where h is the Stieltjes function, other examples are the function s of Theorem 2, or e^{-x}, which is not Stieltjes.

Because our goal is to improve the approximation of a smooth function f, the second property required for the reference function s is to be characterized by the same kind of smoothness as f. All functions presented in this paper are “convex-like”, i.e., the difference between such function and a convex function on the considered interval is negligible.

For instance, the interesting suggestion by Claude Brezinski to use a Hermite interpolation polynomial of f as a reference function s failed (see table of Section 3): this polynomial is not sufficiently smooth and, both s_1 and s_2 can be either larger or smaller than s, rather than being on the opposite sides of s (the property TSE is not satisfied).

The accuracy of the weighted approximation is quite sensitive to the proximity of reference function s to approximated function f. Since the process of selection of the suitable reference function is largely "experimental" it is desirable to have a number of choices for s.

Choice of NPA. The two sided estimates may be obtained not only by using $[k/k]$ and $[k-1/k]$ NPAs. Other NPAs $[m/n]$ and $[m-1/n]$ can be used as well. For instance, in the following we successfully use the NPAs $[2/3]$ and $[1/3]$. The next question concerns the choice of m and n for NPAs. For this purpose we can use the same procedures as those used for selecting the best PA largely presented in [2, 3] for the ordinary one-point PA.

Rescaling. To preserve the Stieltjes character of s one must restrict the transformation of Stieltjes function h to the following:

$$s(x) = c \times h(ax + b). \tag{11}$$

Here we have a degree of flexibility: the three parameters being subject to only two conditions (9). Occasionally the calculated parameters a, b, c can be extremely large. In such cases, we may select just one condition listed in (9), or give up the Stieltjes character of s. We found the following rescaling quite effective:

$$s(x) = (ax + b) \times h(cx + d). \tag{12}$$

To assure that reference function s is as close as possible to f, we can use some global condition minimizing the distances between s and f. We can also use a simple condition at one point x^* of interval $[x_1, x_N]$:

$$s(x^*) = f(x^*) \tag{13}$$

in cases when we know the value $f(x^*)$.

Calculation of the weights $\boldsymbol{\alpha_i}$. In practical calculation we select the middle point of each interval to obtain the inequality for α_i from (7). We observed a number of times that $\alpha_i/(1-\alpha_i) \gg 1$ and f is not necessarily close to s. Consequently the result is not certain a priori and in some cases the approximations m_i can be worse than f_1. Fortunately this arises quite seldom and is usually limited to one among $N-1$ subintervals.

Somewhat simplified version of the presented method of approximation can be reduced to a calculation of the mean $\overline{\alpha}$ of all weights:

$$\overline{\alpha} = (\alpha_1 + \alpha_2 + \ldots + \alpha_{N-1})/(N-1)$$

allowing us to define a global approximation

$$m = \overline{\alpha} f_1 + (1 - \overline{\alpha}) f_2. \tag{14}$$

Our examples show that this method may work equally well.

3. Approximation of $f(x) = e^{-x}/x$. In this example we use the following information at four points $x = 2, 4, 6, 8$: $f(x_1)$, $f'(x_1)$, $f''(x_1)$, $f(x_2)$, $f(x_3)$, $f(x_4)$ to compute the NPAs $f_1 = [2/3]_{2468}^{3111}$ and $f_2 = [1/3]_{2468}^{2111}$. The Stieltjes function $h(x) = \frac{1}{x}\log(x)$ is used to obtain the reference function s rescaled by (9) and (13):

$$s(x) = (-.016247x + .130118)\frac{\log(x)}{x-1}. \tag{15}$$

The inequality (7) leads to the inequalities $\alpha_i > A_i$. The calculations were performed with:

x	A_i	α_i
3	.93403	.967015
5	.895191	.947596
7	.8883	.944152

It is not surprising that the “bad” NPA $f_2 = [1/3]$ contributes less then 5% to the approximation. In the next table we present the numerical results. Recall that m_i in the second column correspond to the local approximations on the intervals $[2i, 2(i+1)]$, $i = 1, 2, 3$, and the third column corresponds to the approximation m (14) computed with the mean weight $\alpha = .952921$.

If we use the Hermite polynomials of interpolation H built using all available data for f as the reference function s, then clearly $s_1 = f_1$ and $s_2 = f_2$, so our weighted approximation becomes identical to s which is not convex-like, not sufficiently smooth (Fig. 1). We see that the result is quite poor (fourth column). It is not surprising since in most cases the Hermite polynomial of interpolation does not have the TSE property because s_1 and s_2 are frequently on the same side of s, as shown in two last columns (Fig. 2).

x	$f - f_1$	$f - m_i$	$f - m$	$f - H$	$H - f_1$	$H - f_2$
2	.0	.0	.0	.0	.0	.0
2.5	.000072	$-.000084$	$-.00015$	$-.00091$	.00098	$-.00374$
3	.0001	.000001	$-.000046$	$-.00312$	.00323	$-.00013$
3.5	.000058	.000027	.000014	$-.00337$	.00343	.00250
4	.0	.0	.0	.0	.0	.0
4.5	$-.000026$	$-.000017$	$-.000018$	.00562	$-.00565$	$-.00548$
5	$-.000025$	$-.000019$	$-.000020$	.00996	$-.00999$	$-.00987$
5.5	$-.000013$	$-.0000108$	$-.0000110$	.00896	$-.00898$	$-.00893$
6	.0	.0	.0	.0	.0	.0
6.5	.0000087	.0000075	.0000077	$-.01604$	.01605	.01603
7	.000011	.0000099	.000010	$-.03263$	.03264	.03262
7.5	.0000079	.0000071	.0000072	$-.03540$	.03541	.03539
8	.0	.0	.0	.0	.0	.0

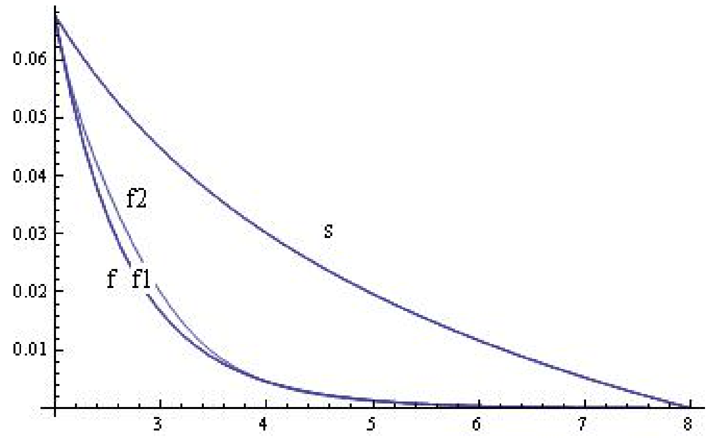

Fig. 1. In this scale f and f_1 seem superposed. In spite of the distance between f and s weights calculated for s result in excellent approximation of f.

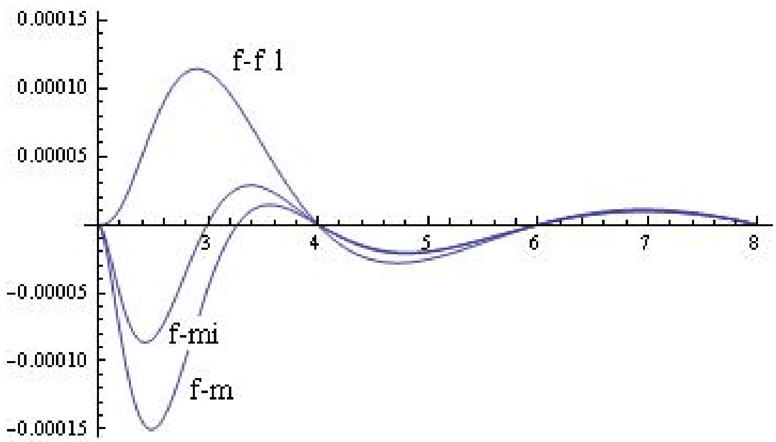

Fig. 2. Errors of approximations with reference to (15). Approximation m_i is approximately 5 times better than f_1.

Notice, that only at the point $x = 2.5$ the NPA f_1 is a little better than m_1, but m at this point is rather poor.

Respecting the Stieltjes property of s and using the rescaling (11) with $c = 1$ we obtain the following reference function:

$$s(x) = \frac{\log(50127.x - 100191)}{50127.x - 100192}, \tag{16}$$

Using the mean weights $m = .629645 f_1 + .370356 f_2$ we get (Fig. 3)

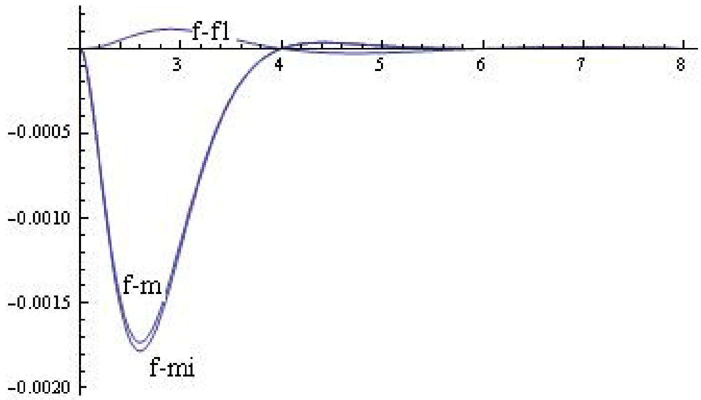

Fig. 3. Errors of approximations with reference to (16). Note that here the scale is multiplied by 10 with respect to Fig. 2. This illustrates why the choice of the reference function and its rescaling must be very careful.

x	$f - f_1$	$f - m_i$	$f - m$
2	.0	.0	.0
2.5	.0000718	−.001723	−.00167
3	.00011	−.00117	−.0011
3.5	.000058	−.000296	−.00029
4	.0	.0	.0
4.5	−.000026	.000035	.000034
5	−.0000251	.000018	.000017
5.5	−.000013	.0000041	.0000038
6	.0	.0	.0
6.5	.0000087	.0000012	.00000091
7	.000011	.0000028	.0000024
7.5	.0000079	.0000026	.0000023
8	.0	.0	.0

4. Approximation of $f(x) = e^{-x}$. The enormous coefficients in the last rescaled function s suggest the need to restrict the adjustment of s and f to one point $x = 2$ and to manipulate three coefficients a, b, c in (11). As in the last example we consider four points 2, 4, 6, 8. The reference function becomes simpler, namely:

$$.303\frac{\log(2x)}{2x-1}. \tag{17}$$

Using the same notations as previously $f_1 = [2/3]$, $f_2 = [1/3]$ and $m = .875895f_1 + .1241045f_2$ we obtain (Fig. 4)

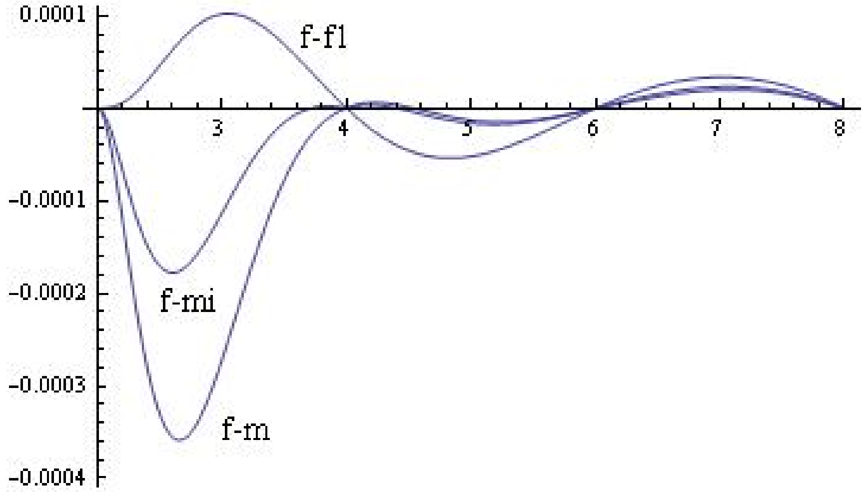

Fig. 4. Errors of approximations with reference to (17). Observe the quality of m_i and m with respect to f_1 for $x > 3.5$. The NPA f_1 is a little better than m_1 only at point $x = 3$.

x	$f - f_1$	$f - m_i$	$f - m$
2	.0	.0	.0
2.5	.000047	$-.00017$	$-.00033$
3	.000102	$-.000112$	.00027
3.5	.000069	$-.000015$	$-.000077$
4	.0	.0	.0
4.5	$-.000046$	.0000013	$-.0000028$
5	$-.000052$	$-.000013$	$-.000016$
5.5	$-.0000305$	$-.000013$	$-.000014$
6	.0	.0	.0
6.5	.000024	.0000126	.0000155
7	.000025	.0000197	.000023
7.5	.000025	.000016	.000018
8	.0	.0	.0

5. Approximation of gaussian distribution from the tribology problem. This practical problem prompted us to take a look at different methods of approximation. The following integral of the Gaussian distribution of asperity heights x in the tribology model of contact of two surfaces appears in many calculus problems [6] :

$$g(x) = \frac{1}{\sqrt{2\pi}} e^{\frac{x^2}{2}} \int_x^\infty (s - x)^{\frac{5}{2}} e^{-\frac{s^2}{2}} ds. \tag{18}$$

A number of analytical formulas for g based on the tabulated numerical values of g have been published, however, as we demonstrated in [7] the simple Padé approximation gives more accurate

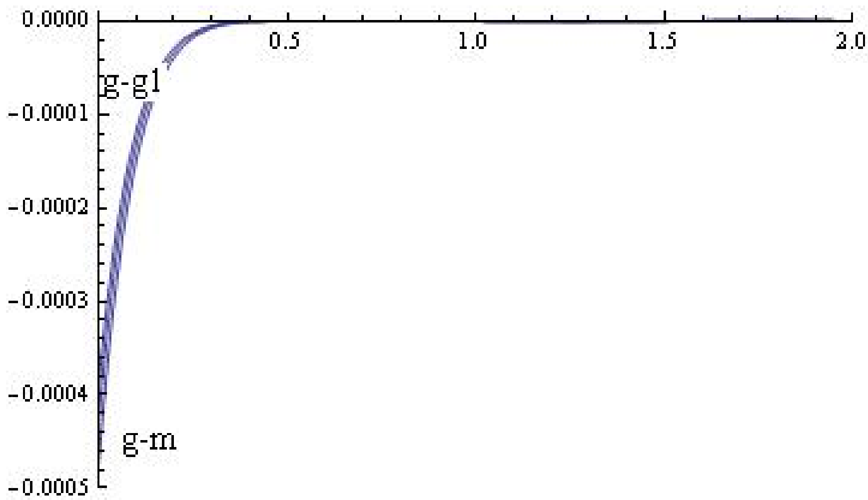

Fig. 5. Errors of approximations with reference to (19). A little superiority of m_i and m with over g_1 is hardly detectable on this graph.

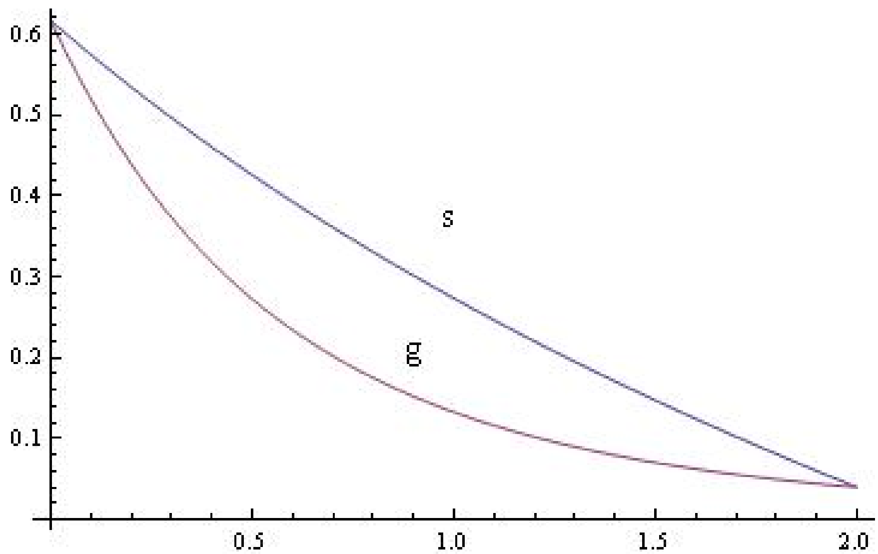

Fig. 6. Characteristic gap between approximated function g and reference function s.

results than all previously proposed formulas. As demonstrated below, the accuracy can be further improved by using the method presented here. Following Greenwood we consider five values of g in the interval $[0, 2]$. $g(0) = .62$, $g(2) = .04$. For $x > 2$. g is very close to 0: $g(x) < .001$. The Stieltjes function $\frac{1}{x}\log(1 + x)$ rescaled following (9) at $x = 0$ and $x = 2$, and (12) leads to the reference function

$$s(x) = \frac{\log\left(\dfrac{x}{2} + 1\right)}{\dfrac{x}{2}}(-.279408x + .616634). \tag{19}$$

The considered four points are .5; 1; 1.5; 2 (Figs. 5 and 6). The NPAs, as previously, are $g_1 = [2/3]$ and $g_2 = [1/3]$. The weights computed at .75; 1.25; 1.75 are $\alpha_1 = .992$, $\alpha_2 = .982$ and $\alpha_3 = .974$. The weighted mean is $m = .982725g_1 + .017275g_2$.

Computed values of g and s used to obtain the approximation formulas and errors of approximations

x	g	s	$g - g_1$	$g - m_i$	$g - m$
.0	.616634	.616634	−.00039	−.00043	−.00048
.25	.0404421	.515213	−.0000126	−.000015	−.000018
.5	.272411	.425695	.0	.0	.0
.75	.188069	.345695	.00000046	.00000038	.00000027
1	.132825	.273467	.0	.0	.0
1.25	.0957906	.207699	−.00000076	−.00000065	−.00000066
1.5	.0704232	.147382	.0	.0	.0
1.75	.0526961	.0917191	.0000012	.0000011	.0000011
2	.0400761	.0400761	.0	.0	.0

6. Conclusion. The presented method is based on a novel idea of constructing the weighted mean approximation of a given function of interest by first determining a similar weighted approximation of a known function. The accuracy of the approximation is sensitive to the proximity of the two functions. Efficient use of the method requires that a rather large collection of reference functions having the TSE property is available, this will happen with a wider use. A few examples presented here clearly demonstrate that the idea is very promising, opening an exciting area for further investigation in the numerical approximation of functions.

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