Adaptive point shifts in rational approximation with optimized denominator[☆]

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Abstract

Classical rational interpolation is known to suffer from several drawbacks, such as unattainable points and randomly located poles for a small number of nodes, as well as an erratic behavior of the error as this number grows larger. In a former article, we have suggested to obtain rational interpolants by a procedure that attaches optimally placed poles to the interpolating polynomial, using the barycentric representation of the interpolants. In order to improve upon the condition of the derivatives in the solution of differential equations, we have then experimented with a conformal point shift suggested by Kosloff and Tal-Ezer. As it turned out, such shifts can achieve a spectacular improvement in the quality of the approximation itself for functions with a large gradient in the center of the interval. This leads us to the present work which combines the pole attachment method with shifts optimally adjusted to the interpolated function. Such shifts are also constructed for functions with several shocks away from the extremities of the interval.

MSC: 65D05; 41A20; 41A05

Keywords: Rational approximation; Interpolation; Optimal interpolation; Point shifts

1. Introduction

Our aim in the present work is the rational approximation of a function f on a real interval I, which we may take as $[-1, 1]$ without loss of generality, in such a way that the approximant interpolates f between $N + 1$ abscissae $x_0, \ldots, x_N$ in I which are either given in advance or images

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of given points under a conformal map. The reader may consult [6] for an example of an application of such interpolants. We assume that f is analytic (holomorphic) within a domain $\mathscr{D}_1$ containing I.

Let p_N be the polynomial of degree at most N interpolating f between $x_0, \ldots, x_N$. It is well known that, for good interpolation points (nodes) such as Chebyshev's or Legendre's, one has exponential convergence of the sequence p_N toward f:

$$|p_N - f| \leqslant c \cdot \mathrm{e}^{-\alpha N}$$

for some constants c and α. (This same kind of interpolation is also of interest if f is merely in $C^{p-1}(I)$ for large p with $f^{(p)}$ of bounded variation, in which case one reaches an order of convergence p:

$$|p_N - f| \leqslant c \cdot N^{-p}.)$$

However, the constants c and α in the above estimate depend, explicitly or implicitly, on derivatives of f; when the latter are very large, the fast convergence may show up only after too large values of N for practical purposes.

Rational interpolation often does much better for small values of N. However, classical rational interpolants r, in which the sum of the degrees of numerator and denominator add up to N, are unpredictable for small N. In many cases, which document more the rule than the exception, unwanted poles occur in the vicinity of I, or even on I, making the corresponding r useless as approximants.

To obtain better interpolants r in cases f is known everywhere on I, we have proposed in [5] to attach poles to p_N in such a way as to minimize some functional, e.g., some norm $\|r - f\|$, taken as a measure of the approximation error. The decrease of the functional induced by the optimization documents the motion of the poles from their position at infinity (for p_N) to an optimal finite position. In sharp contrast to classical interpolants, the resulting rational interpolants r are at least as good as p_N and neither unwanted poles nor unattainable points [18] may occur.

Quite impressive results have been obtained in [5] with this method, and this even with equidistant x_k, for which p_N is notoriously useless for many f when N grows large (Runge's phenomenon). For these points the computations had however to be performed in quadruple precision (about 32 digits), a manifestation of the ill-conditioning. And the higher N, the higher the necessary precision.

If the goal is just to approximate f, and if one can choose the x_k—a situation we will assume here—it is clearly better to stay with Chebyshev or Legendre points. On the other hand, it is well known by experts in spectral methods that derivatives of polynomials interpolating between such points which accumulate in the vicinity of the boundary are ill-conditioned for large N. Kosloff and Tal-Ezer [14] have therefore suggested to conformally shift these points from their, say, Chebyshev position by a conformal map g from a y-domain containing another copy J of I (with the Chebyshev points y_k) onto a domain containing $\mathscr{D}_1$, and this in such a way that $g(J) = I$ and that the new nodes $x_k = g(y_k)$ are closer to equidistant than the y_k's. These authors then suggest to approximate f by the transplant of the polynomial in y of degree at most N interpolating $F(y) := f(x)$ between the y_k. While the exponential convergence is maintained by the analyticity of g, the derivatives are now better conditioned.

We have successfully applied that same idea in [7] to our rational interpolant with optimized poles of [5]. As a by-product, the improvement in the approximation was particularly impressive for functions with a large gradient in the center of the interval, a consequence of the fact that Kosloff and Tal-Ezer's shift places more nodes there. Though not surprising in principle, this improvement

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impressed us by its magnitude: in some cases it was more pronounced than that obtained from the attachment of poles.

After having studied the numerical results of [7], Richard Baltensperger has suggested that we use instead of Kosloff and Tal-Ezer's shift a much more adaptive g such as the one advocated and proven more efficient and versatile by Bayliss and Turkel in [2]. The present work is devoted to the use of such adaptive point shifts for improving upon the optimized denominator rational interpolation of [5].

Section 2 reviews polynomial interpolation and the method of constructing rational interpolants by optimally attaching poles to the interpolating polynomial, as introduced in our earlier work. Section 3 recalls the effect of conformal point shifts on the interpolant and its derivatives. Section 4 describes the use of Bayliss and Turkel's point shift, which involves two parameters, one for the location of an accumulation of points, the other for their concentration. In Section 5 we construct a new shift that can in principle handle an arbitrary number of shocks. The work is completed with numerical examples and conclusions.

2. Rational interpolation with optimized denominator

This interpolation method, recently introduced in [5], starts with the polynomial interpolant. The unique polynomial p_N of degree $\leqslant N$ that interpolates f between the x_k may be written in its *barycentric form* [13]

$$p_N(x) = \sum_{k=0}^{N} \frac{w_k}{x - x_k} f_k \left/ \sum_{k=0}^{N} \frac{w_k}{x - x_k} \right. , \qquad (2.1)$$

where

$$w_k := 1 \left/ \prod_{i=0, i \neq k}^{N} (x_k - x_i) \right. .$$

For several standard point sets $\{x_k\}_{k=0}^{N}$, the *weights* w_k may be analytically computed, one of the many advantages of Lagrange interpolation [3]. This is in particular the case for Chebyshev points. Moreover, since the w_k appears in the numerator and in the denominator of (2.1), any common factor may be discarded. Here we will use the Chebyshev points of the second kind $x_k = \cos k\pi/n$, whose simplified weights read [17]

$$w_k^* = (-1)^k \delta_k, \quad \delta_k := \begin{cases} 1/2, & k = 0 \text{ or } k = N, \\ 1 & \text{otherwise.} \end{cases}$$

Then (2.1) evaluates p_N at any given x in $\mathcal{O}(N)$ operations.

As mentioned in the Introduction, the convergence $p_N \to f$ is very rapid if f is differentiable a large number p of times, and it adapts automatically to p. It is exponential for analytic functions such as those we will consider in the examples.

On the other hand, it is easy to infer from Markov's inequality that, when functions with steep gradients (shocks) are to be approximated, the degree N, and hence the number of x_k, will have to grow sharply with the steepness of the shocks [5]. Rational interpolation is thus to be preferred

when approximating functions with large slopes. As mentioned in the Introduction, classical rational interpolation is hampered by unattainable points and unpredictable poles close to or even on I (see, e.g., Fig. 1b and Table 5 in [5]).

For this reason, we have suggested in [5] a different kind of rational interpolation in cases where f is known everywhere on I and where the computing time is not an issue. The basic idea is to start with p_N, which may be viewed as a rational interpolant with all its poles at infinity, to fix P, the number of poles z_j to be attached to p_N, and to move the z_j from infinity toward an optimal position, i.e., one which minimizes some error functional, here $\|r - f\|_\infty$.

Let $\mathscr{R}_{mn}$ denote the set of all rational functions with numerator and denominator degrees at most m, resp. n. Our problem is therefore the following.

Problem. Find among all $r \in \mathscr{R}_{NP}$ with $r(x_k) = f(x_k)$, $k = 0, 1, \ldots, N$, one that minimizes

$$\|r - f\|_\infty := \max_{x \in I} |r(x) - f(x)|. \tag{2.2}$$

It is easy to see that this optimization problem has a solution [5]. The unicity question is not settled, yet.

The resulting interpolants have many advantages over classical rational interpolants: they can have neither unattainable points nor unwanted poles, and the sequence $\{\|r - f\|_\infty : r \in \mathscr{R}_{NP}\}$ decreases as P increases.

The barycentric representation of p_N permits a very simple attachment of the poles: it suffices to replace the w_k in (2.1) with

$$b_k := w_k \cdot d_k, \quad d_k := \prod_{i=1}^{P} (x_k - z_i) \tag{2.3}$$

(if an interpolant with the poles z_j exists, see [5]). The optimization problem has been numerically solved with success in [5] with standard modern algorithms. The results show that the nice properties just mentioned also arise in practice, and in particular that the resulting interpolants can indeed accommodate much more pronounced shocks than p_N.

In [6], such optimized rational interpolants have been computed as one part of a two-step algorithm for improving upon the polynomial pseudospectral solution of two-point boundary value problems. There, the minimized error functional was the size of the residual of the differential equation for the approximate solution r. This residual involves derivatives, which are notoriously ill-conditioned for large number N of Chebyshev—or Legendre—points [20].

3. Conformal points shifts and their influence upon the derivatives

To reduce the just-mentioned ill-conditioning, Kosloff and Tal-Ezer [14] have suggested using in lieu of the Chebyshev points themselves their images under a conformal map that renders them closer to equidistant, an idea which has proven effective in several instances [1,4,15,16]. We have applied it ourselves in [7] to the above method of interpolation with optimized denominator.

There we have attached poles z_j in x-space by attaching poles $v_j = g^{[-1]}(z_j)$ to $P_N(y) = \sum_{k=0}^{N} (w_k/(y - y_k)) f_k / \sum_{k=0}^{N} (w_k/(y - y_k))$ in y-space. In view of (2.3), the resulting rational

interpolant reads

$$R(y) := \frac{\displaystyle\sum_{k=0}^{N} \frac{w_k \prod_{i=1}^{P}(y_k-v_i)}{y-y_k} f_k}{\displaystyle\sum_{k=0}^{N} \frac{w_k \prod_{i=1}^{P}(y_k-v_i)}{y-y_k}} = \frac{\displaystyle\sum_{k=0}^{N} \frac{w_k \prod_{i=1}^{P}(g^{[-1]}(x_k)-g^{[-1]}(z_i))}{g^{[-1\ ]}(x)-g^{[-1]}(x_k)} f_k}{\displaystyle\sum_{k=0}^{N} \frac{w_k \prod_{i=1}^{P}(g^{[-1]}(x_k)-g^{[-1]}(z_i))}{g^{[-1\ ]}(x)-g^{[-1]}(x_k)}} =: r(x)$$

and the v_j are optimized by minimizing

$$\|R - F\|_\infty = \max_{y \in J} |R(y) - F(y)|, \tag{3.1}$$

as in (2.2).

As mentioned in the Introduction, one goal of the conformal shift, besides a better approximation at steep shocks in the interior of the interval, is the improvement of the approximation of the derivatives. The derivatives of r are given as functions of those of R by [7]

$$r'(x) = R'(y)y'(x) = \frac{R'(y)}{g'(y)}$$

$$r''(x) = R''(y)[y'(x)]^2 + R'(y)y''(x) = \frac{R''(y)}{[g'(y)]^2} - \frac{g''(y)}{[g'(y)]^3} R'(y), \tag{3.2}$$

where the derivatives of

$$R(y) = \sum_{k=0}^{N} \frac{u_k}{y-y_k} f_k \left/ \sum_{k=0}^{N} \frac{u_k}{y-y_k}\right.$$

can be computed by the Schneider–Werner formulae

$$R'(y) = \begin{cases} \displaystyle\sum_{k=0}^{N} \frac{u_k}{y-y_k} R[y,y_k] \left/ \sum_{k=0}^{N} \frac{u_k}{y-y_k}\right. , & y \neq y_i, \ i=0(1)N, \\[3ex] -\left(\displaystyle\sum_{k=0,k\neq i}^{N} u_k R[y_i,y_k]\right) \left/ u_i\right. , & y = y_i, \end{cases}$$

$$R''(y) = \begin{cases} 2\displaystyle\sum_{k=0}^{N} \frac{u_k}{y-y_k} R[y,y,y_k] \left/ \sum_{k=0}^{N} \frac{u_k}{y-y_k}\right. , & y \neq y_i, \ i=0(1)N, \\[3ex] -2\left(\displaystyle\sum_{k=0,k\neq i}^{N} u_k R[y_i,y_i,y_k]\right) \left/ u_i\right. , & y = y_i, \end{cases}$$

with $R[z,z,y_k] = (R'(z) - R[z,y_k])/(z - y_k)$.

4. Adaptive point shifts for functions with a shock

It now remains to choose a good conformal point shift g. In [7], we went for Kosloff and Tal-Ezer's map,

$$g(z) = \frac{\arcsin \alpha z}{\arcsin \alpha}$$

with a parameter α varying from 0 to 1. For $\alpha = 0$, the points remain the Chebyshev ones. As $\alpha \to 1$ they become equidistant. The fast convergence rates mentioned in the Introduction are maintained for every fixed $\alpha < 1$.

This shift was introduced for improving the conditioning of the derivatives of the approximation in time evolution problems. In [7], however, we have noticed an important by-product, namely a sharp improvement in the quality of the approximation itself for functions with a shock at 0. The aim of the present work is to take a better advantage of this effect by adapting the shift to the interpolated function. We achieve this by considering the various proposals for shifts g by Bayliss and Turkel in [2]. Their comparisons demonstrate the particularly remarkable efficiency of the map

$$x = g(y) = \frac{1}{\alpha} \tan[\lambda(y - \mu)] + \beta, \tag{4.1}$$

where

$$\lambda = \frac{\gamma + \delta}{2}, \quad \mu = \frac{\gamma - \delta}{\gamma + \delta} \tag{4.2}$$

with

$$\gamma = \arctan[\alpha(1 + \beta)], \quad \delta = \arctan[\alpha(1 - \beta)].$$

g embodies two parameters: β determines the location of the maximal gradient, α its magnitude, (g is constructed from $y = g^{[-1]}(x) = \mu + (1/\lambda)\arctan[\alpha(x - \beta)]$, and β is the location of the maximal gradient of the corresponding arcus tangens; notice that $\mu = 0$ for $\beta = 0$.) Fig. 1b displays $g^{[-1]}(x)$ for $\alpha = 35.35$ and $\beta = -0.5024$, the best values for approximation without the help of poles in Table 2 (Example 1).

Bayliss and Turkel have roughly optimized the shift by computing over a grid of values of α and β and selecting those parameter values for which a functional related to the interpolation error is minimized. Here we minimize the functional (3.1) with respect to the $P + 2$ variables $z_1, \ldots, z_P, \alpha, \beta$ using standard software. In the numerical examples discussed in Section 6, we also estimate the precision of the derivatives of r by evaluating $\|r' - f'\|_\infty$ and $\|r'' - f''\|_\infty$ with the formulae (3.2). A simple calculus exercise yields for the expressions containing g:

$$g'(y) = \alpha \cos^2 t / \lambda, \quad \frac{g''(y)}{[g'(y)]^3} = 2\alpha^2 \cos^3 t \sin t / \lambda, \quad t = \lambda(y - \mu).$$

Notice that, in contrast with the method used in [5–7], the nodes x_k are no longer chosen at the onset, but result from the optimization procedure. The Remes algorithm [8], on the other hand, yields best rational approximants in $\mathscr{R}_{N,P}$ which interpolate between (at least) $N + P + 2$ abscissae x_k. Our x_k, however, have the advantage of being images of fixed points y_k under a conformal map determined by only few parameters.
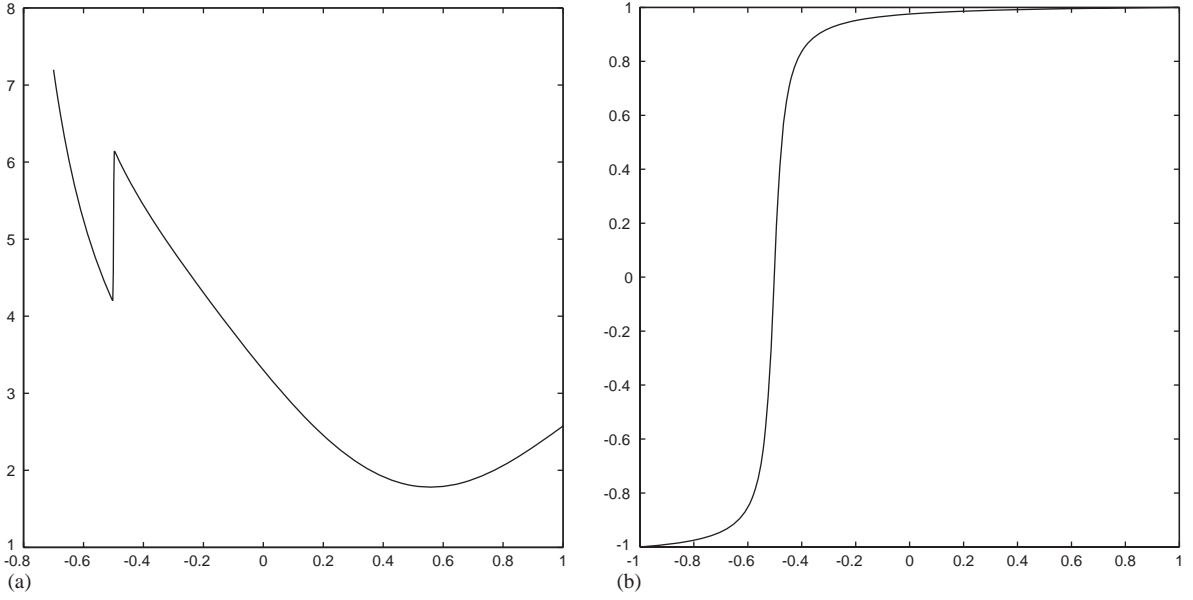
Fig. 1. Function and inverse change of variable $y = g^{[-1]}(x)$ in Example 1, Table 2, no poles.

5. Functions with multiple shocks

After having addressed functions with one steep gradient in the interior of I, it is natural to consider functions f with several such shocks. When these are sufficiently close to one another, a simple change of variable with two parameters as in (4.1) will sometimes do [2]. In more general cases, however, two parameters will be necessary for every shock (one for location, the other for steepness).

One way is to split I into subdomains and to consider another approximation on each of them [2]. This, though, ruins the spectral accuracy.

It therefore seems preferable to address such problems with a single conformal map involving two parameters for every shock, say α_q and β_q. We will now construct such a map. The basic idea arises from the observation that, as $g^{[-1]}$ in (4.1) is steep at the shock, it is relatively flat away from the latter, and the more so the steeper the shock. At such flat parts one thus can *add* another function to $g^{[-1]}$ without altering it too much. We therefore construct a new $g^{[-1]}$ accommodating Q shocks as

$$y(x) = g^{[-1]}(x) = \mu + \frac{1}{\lambda} \sum_{q=1}^{Q} \arctan[\alpha_q(x - \beta_q)], \tag{5.1}$$

where λ and μ are the parameters needed for ensuring that $g^{[-1]}(-1) = -1, g^{[-1]}(1) = 1$. A straightforward solution of this 2×2-system yields the same values of λ and μ as in (4.2), with

$$\gamma := \sum_{q=1}^{Q} \arctan[\alpha_q(1 + \beta_q)],$$

$$\delta := \sum_{q=1}^{Q} \arctan[\alpha_q(1 - \beta_q)].$$

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To find g itself, we notice that $g^{[-1]}$, as a sum of monotone increasing functions, is itself monotone increasing from -1 to 1 and that, consequently, the equation $g^{[-1]}(x) = y$, i.e.,

$$\sum_{q=1}^{Q} \arctan[\alpha_q(x - \beta_q)] = \lambda(y - \mu) \tag{5.2}$$

has a solution x for every $y \in J$. The sum of arcus tangens may be written as a single arcus tangens, the argument of which is a rational function involving x^Q. (5.2) thus will in general require a numerical solution, e.g., with the method of Dekker–Brent [9]. For $Q \leqslant 4$, y may be expressed according to the formulae for roots of polynomials. For simplicity, we will confine ourselves here to the case $Q = 2$. Eq. (5.2) then yields

$$\frac{\alpha_1(x - \beta_1) + \alpha_2(x - \beta_2)}{1 - [\alpha_1\alpha_2(x - \beta_1)(x - \beta_2)]} = \tan[\lambda(y - \mu)] =: t \tag{5.3}$$

or $ax^2 + bx + c = 0$ with

$$a := \alpha_1\alpha_2 t, \quad b := [(\alpha_1 + \alpha_2) - a(\beta_1 + \beta_2)],$$

$$c := (\alpha_1\alpha_2\beta_1\beta_2 - 1)t - (\alpha_1\beta_1 + \alpha_2\beta_2).$$

Notice that the sum formula used to transform (5.2) into (5.3) holds true merely up to multiples of π. We have therefore chosen that solution of the quadratic equation for which $g^{[-1]}(x)$ equals y, the value to be inverted.

The derivatives, to be inserted into (3.2) when computing $r'(x)$ and $r''(x)$, are obviously given by

$$y'(x) = \frac{1}{\lambda} \sum_{q=1}^{Q} \frac{\alpha_q}{1 + s_q^2},$$

$$y''(x) = \frac{-1}{\lambda} \sum_{q=1}^{Q} \frac{2\alpha_q^2 s_q}{(1 + s_q^2)^2}, \quad s_q := \alpha_q(x - \beta_q).$$

6. Numerical examples

We have tested the effect of adaptive point shifts on our rational interpolation with optimized poles on two examples, one with a single shock, the other with two shocks. The optimization problems were solved with the simulated annealing method of [11]. The minimized sup-norm (3.1) has thereby been estimated by considering the 1000 equally spaced points

$$\hat{y}_\ell = -\frac{5}{4} + \frac{\ell - 1}{999} \frac{10}{4}, \quad \ell = 1(1)1000,$$

on the interval $[-5/4, 5/4]$ and computing the maximal absolute value of the error at those $\hat{y}_\ell$ lying in $[-1, 1]$.

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Table 1

Effect of an optimized Bayliss–Turkel point shift on rational approximation with optimized poles in Example 1 with $\varepsilon = 10'000$ and $N = 100$

β	α	Poles	$\|r - f\|$	$\|r' - f'\|$	$\|r'' - f''\|$
*	*		1.684e − 1	2.214e + 1	6.027e + 3
*	*	$(-0.4902, \pm 2.011e - 2)$	5.224e − 4	2.158e − 1	8.241e + 1
		$(-0.5056, \pm 2.228e - 2)$			
		$(-0.5178, \pm 5.613e - 2)$			
−0.5185	7.408		9.447e − 9	5.012e − 6	1.138e − 2
−0.4976	8.273	$(-1.027, \pm 3.147e - 3)$	1.279e − 11	6.270e − 9	1.654e − 5
−0.4981	8.519	$(-1.030, \pm 3.574e - 3)$	2.495e − 12	1.754e − 9	5.659e − 6
		$(1.062, \pm 5.346e - 3)$			

Table 2

Effect of an optimized Bayliss–Turkel point shift on rational approximation with optimized poles in Example 1 with $\varepsilon = 1'000'000$ and $N = 240$

β	α	Poles	$\|r - f\|$	$\|r' - f'\|$	$\|r'' - f''\|$
*	*		7.076e−1	4.803e + 2	4.504e + 5
*	*	$(-0.5001, \pm 2.017e - 3)$	8.031e − 4	2.628e + 1	4.491e + 4
		$(-0.5041, \pm 2.080e - 2)$			
		$(-0.5012, \pm 8.379e - 3)$			
−0.5024	35.35		2.873e − 9	2.335e − 5	8.499e − 2
−0.5009	39.79	$(-1.007, \pm 9.506e - 4)$	6.340e − 11	2.466e − 7	2.431e − 3
−0.4968	42.59	$(-1.006, \pm 6.682e - 4)$	4.860e − 12	4.062e − 8	2.151e − 3
		$(1.046, \pm 6.790e - 3)$			

Example 1. The function is

$$f(x) = e^{1/(x+1.2)} + \cos \pi(x + 0.5) + \frac{\mathrm{erf}(\delta(x + 0.5))}{\mathrm{erf}(\delta)}, \quad \delta = \sqrt{0.5\varepsilon}.$$

It consists of a function suggested in [12] as a test for solution methods for two-point boundary value problems, shifted by -0.5 and supplemented with a term with essential singularity at $x = -1.2$, i.e., on the real axis to the left of I. Fig. 1a shows f for $\varepsilon = 10^6$ between -0.7 and 1, in order for the shock to be distinguishable (at -1 the value of f is about 147).

First, we have approximated f for $\varepsilon = 10'000$. The results with $N = 100$ are displayed in Table 1. β and α are the parameters used in the change of variable (4.1)—stars thereby meaning that no change is made—the third column gives the optimized pole pairs and the last three show the approximation errors $\|r - f\|$, $\|r' - f'\|$ and $\|r'' - f''\|$, estimated in the same way as the minimized norms (3.1)—but now in x-space with equidistant $\hat{x}_\ell := \hat{y}_\ell$.

Table 1 documents the successive improvements in the approximation: the polynomial has an error of about 10^{-1}, which decreases to $5 \cdot 10^{-4}$ with the attachment of six poles. Without poles, on the other hand, but with an optimized Bayliss–Turkel point shift (4.1), the error becomes as small as 10^{-8}!

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Table 3

Effect of an optimized two-shock point shift on the rational approximation with optimized poles in Example 2 with $\varepsilon = 10'000$, $\eta = 100$ and $N = 200$

β_1	α_1	β_2	α_2	Poles	$\|r - f\|$	$\|r' - f'\|$	$\|r'' - f''\|$
*	*	*	*		$4.441\mathrm{e} - 2$	$1.175\mathrm{e} + 1$	$3.096\mathrm{e} + 3$
*	*	*	*	$(-0.5000, \pm 1.572\mathrm{e} - 2)$ $(0.7293, \pm 7.826\mathrm{e} - 2)$ $(0.7494, \pm 3.717\mathrm{e} - 2)$	$1.109\mathrm{e} - 5$	$3.598\mathrm{e} - 3$	1.301
-0.4924	13.25	0.7125	5.114		$1.728\mathrm{e} - 8$	$2.022\mathrm{e} - 5$	$2.151\mathrm{e} - 2$
-0.4819	15.40	0.7141	5.777	$(0.1010, \pm 7.037\mathrm{e} - 2)$	$1.667\mathrm{e} - 9$	$4.097\mathrm{e} - 6$	$3.066\mathrm{e} - 3$
-0.4855	15.41	0.7154	4.888	$(0.1199, \pm 8.128\mathrm{e} - 2)$ $(0.7084, \pm 1.048\mathrm{e} - 1)$	$1.363\mathrm{e} - 9$	$2.191\mathrm{e} - 6$	$1.577\mathrm{e} - 3$

Shifting to the next order derivative worsens the error by about 10^2 when the precision is low, by 10^3–10^4 when $\|r - f\|$ is small. This is consistent with the theoretical factor for Chebyshev points, about $\mathcal{O}(N)$ in the interior of the interval and $\mathcal{O}(N^2)$ close to the extremities [10]. The factor can therefore be expected to be $\mathcal{O}(N)$ as long as the approximation error—which arises in the interior in our examples—dominates this differentiation error, $\mathcal{O}(N^2)$ when it becomes smaller. Without point shift this derivative-induced loss of accuracy at the end points would be even more pronounced.

For approximating interior shocks, the change of variable is more powerful than the pole attachment; and if it would not be for the function $\mathrm{e}^{1/(x+1.2)}$, attaching poles would not bring much improvement. Because of this steep function outside, but nevertheless close to the approximation interval, the poles are effective here; changes of variable such as (5.1) cannot do any good, they are even harmful since they shift the nodes away from the boundary (this in contrast to the sine-shift used in [19], which on the other hand moves the points away from the interior shocks). The last two examples of Table 1 correspondingly document the efficiency of the pole attachment, with two poles and with four: we end up with a precision of about $2 \cdot 10^{-12}$, with three digits lost for every derivative. The poles come to the vicinity of the boundary.

Similar results were obtained with $\varepsilon = 10^6$, the sole difference being that, due to the larger value of N necessary for a good approximation, the loss in the precision induced by the differentiation is more pronounced, as documented in Table 2 for $N = 240$.

Example 2. Here we started from the above function, shifted by 0.75 instead of -0.5, and we have added to it a tanh-term, centered at -0.5, and the same exponential as before:

$$f(x) = \mathrm{e}^{1/(x+1.2)} + \cos \pi(x - 0.75) + \frac{\mathrm{erf}(\delta(x - 0.75))}{\mathrm{erf}(\delta)} + \tanh(\eta(x + 0.5)), \quad \delta = \sqrt{0.5\varepsilon}.$$

Fig. 2a shows f between -0.7 and 1 for $\varepsilon = 10^4$ and $\eta = 10^2$.

Our results are summarized in Table 3. Without shift the poles come close to the location of the shocks, as in example 1. The point shift is again already impressively efficient without poles. Attaching the latter does not bring too much improvement here. A look at their location reveals that they take care of other difficult stretches than the left boundary layer. Indeed, the first pair
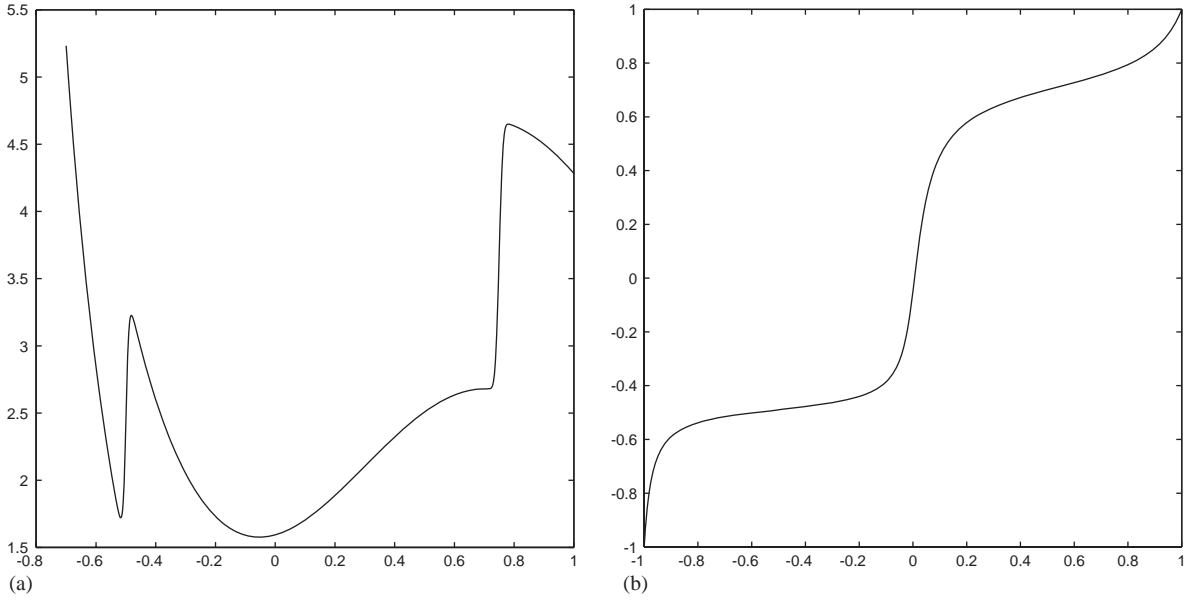
Fig. 2. Function and change of variable $x = g(y)$ in Example 2, Table 3, no poles.

comes close to the median of the location of the two shocks. This may arise from the fact that the concentration of so many points at the shocks depletes the median region too much for a reasonable approximation with the remaining information. The second pair helps at the right shock, which comes so close to 1 (Fig. 2b) that the change of variable cannot move as many points toward it than it does to the left shock. The obtained precision of 10^{-9} is nevertheless quite remarkable for an analytic approximation using "only" 200 interpolation points. And the second derivative stays at a good $1.58 \cdot 10^{-3}$.

7. Conclusion

The combination of adaptive conformal point shifts and optimal pole attachment, as suggested in the present work, turns out to be a very efficient means of improving upon the Chebyshev interpolating polynomial when approximating functions with shocks. We have thereby used a point shift suggested by Bayliss and Turkel before constructing one that can in principle handle a function with an arbitrary number of difficult stretches.

With a single shock, in Example 1, the precision was improved from 10^{-1} to 10^{0} to as much as 10^{-12}, quite an achievement. With two shocks, one of them quite close to the boundary, the error with $N = 200$ worsens to 10^{-9}, but a loss of 10^{-3} for each derivative is very satisfactory for an analytic approximation.

In the future we intend to employ these point shifts for improving upon the two-point boundary value problem solver introduced in [6].

Acknowledgements

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