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The linear rational pseudospectral method with preassigned poles *

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Dedicated to Claude Brezinski on the occasion of his 60th birthday

We present a linear rational pseudospectral (collocation) method with preassigned poles for solving boundary value problems. It consists in attaching poles to the trial polynomial so as to make it a rational interpolant. Its convergence is proved by transforming the problem into an associated boundary value problem. Numerical examples demonstrate that the rational pseudospectral method is often more efficient than the polynomial method.

Keywords: pseudospectral method, linear rational collocation, preassigned poles

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1. Introduction: the problem and the method

The present work will address the solution of linear two-point boundary value problems (BVPs) of the form

$$\begin{aligned} &T[u](x) := u''(x) + p(x)u'(x) + q(x)u(x) = f(x), \quad x \in]-1,1[, \\ &u(-1) = u_{\mathrm{l}}, \qquad u(1) = u_{\mathrm{r}}, \end{aligned} \tag{1}$$

by pseudospectral (or spectral collocation) methods. Spectral methods have been found attractive for solving BVPs as they converge faster than any negative power of the number of points when all arising functions are infinitely differentiable, see, for example, [10,11,14]: they are “spectrally accurate”, therefore often more efficient than finite difference of finite element methods, which converge only at an algebraic rate.

Here we are interested in developing a method that improves upon the pseudospectral (polynomial collocation) method by attaching poles to the trial function so as to make it a rational interpolant. This method is useful when the location of some or all

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of the poles of the solution of the BVP may be determined from the problem, as in equations of Fuchsian type (see [16, p. 370]) or when the BVP is stiff.

The first two authors have already applied rational techniques to partial differential equations [2] and to boundary value problems [7]. However, the (linear) rational pseudospectral method developed in those articles did not take into account the location of the poles of the solution.

Let us first give and alternate presentation of the linear rational pseudospectral method in barycentric form as applied to (1):

1. Choose collocation points x_k, $k = 0(1)N$, and a fixed denominator given in its barycentric form of the first kind [18, p. 106] with respect to the x_k:

$$d(x) = \prod_{j=0}^{N}(x - x_j) \sum_{k=0}^{N} \frac{\beta_k}{x - x_k}. \tag{2}$$

The *weights* β_k determine Lagrange fundamental rational functions

$$L_k^{(\beta)}(x) := \frac{\beta_k/(x - x_k)}{\sum_{i=0}^{N} \beta_i/(x - x_i)},$$

with $L_k^{(\beta)}(x_j) = \delta_{jk}$, where δ_{jk} denotes the Kronecker symbol. The $L_k^{(\beta)}$ span the linear space $\mathcal{R}^{(\beta)}$ of the rational interpolants $\sum_{k=0}^{N} f_k L_k^{(\beta)}(x)$ interpolating values f_k in the x_k. $\mathcal{R}^{(\beta)} \subset \mathcal{R}_{N,N}$, where $\mathcal{R}_{s,t}$ denotes the set of all rational functions with numerator degree less or equal s and denominator degree less or equal t.

2. Replace the solution u in (1) with a rational function in $\mathcal{R}^{(\beta)}$ interpolating between the collocation points x_k, $k = 0(1)N$,

$$u_N(x) := \sum_{k=0}^{N} \tilde{u}_k L_k^{(\beta)}(x). \tag{3}$$

Here we have $\tilde{u}_0 = u_\ell$, $\tilde{u}_N = u_\mathrm{r}$ and the $N-1$ approximations $\tilde{u}_k$ to the $u(x_k)$ remain to be determined.

3. Collocate at the same points x_j, which yields the system of linear equations

$$\sum_{k=0}^{N} \tilde{u}_k L_k^{(\beta)''}(x_j) + p(x_j) \sum_{k=0}^{N} \tilde{u}_k L_k^{(\beta)'}(x_j) + q(x_j) \sum_{k=0}^{N} \tilde{u}_k L_k^{(\beta)}(x_j) = f(x_j),$$
$$j = 1(1)N-1,$$

or in closed form

$$(Tu_N)(x_j) = f(x_j), \quad j = 1(1)N-1. \tag{4}$$

(4) can also be written in matrix form $\mathbf{A}\tilde{\mathbf{u}} = \mathbf{f}$, where $\mathbf{A} := \mathbf{D}^{(2)} + \mathbf{P}\mathbf{D}^{(1)} + \mathbf{Q}$ and

$$\begin{aligned}
&\tilde{\mathbf{u}} := [\tilde{u}_1, \tilde{u}_2, \dots, \tilde{u}_{N-1}]^{\mathrm{T}},\\
&\mathbf{D}^{(1)} = (D_{jk}^{(1)}), \qquad D_{jk}^{(1)} := L_k^{(\beta)\prime}(x_j),\\
&\mathbf{D}^{(2)} = (D_{jk}^{(2)}), \qquad D_{jk}^{(2)} := L_k^{(\beta)\prime\prime}(x_j),\\
&\mathbf{P} := \operatorname{diag}(p(x_j)), \qquad \mathbf{Q} := \operatorname{diag}(q(x_j)),\\
&\mathbf{f} := \big[f(x_j) - u_{\mathrm{r}}\big(D_{j0}^{(2)} + p(x_j)D_{j0}^{(1)}\big) - u_{\mathrm{l}}\big(D_{jN}^{(2)} + p(x_j)D_{jN}^{(1)}\big)\big]^{\mathrm{T}},\\
&\quad j, k = 1(1)N-1.
\end{aligned}$$

(3) is the barycentric form of the interpolating rational function u_N:

$$u_N(x) = \frac{\sum_{k=0}^{N} (\beta_k/(x - x_k))\tilde{u}_k}{\sum_{k=0}^{N} \beta_k/(x - x_k)}. \tag{5}$$

The polynomial interpolant is the special case in which the weights are given (up to a constant) by

$$w_k := \frac{1}{\prod_{j=0, j\neq k}^{N} (x_k - x_j)}, \quad k = 0(1)N,$$

see [15]. For equidistant points, the w_k's are proportional to $(-1)^k\binom{N}{k}$ [15], for Chebyshev points of the second kind $\cos(j\pi/N)$, $j = 0(1)N$, they were found by Salzer [20] to be, again up to a constant,

$$(-1)^k\delta_k, \quad \delta_k := \begin{cases} \dfrac{1}{2}, & k = 0 \text{ or } k = N,\\ 1, & \text{otherwise.} \end{cases} \tag{6}$$

The differentiation matrices $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$ can be given by the formulae (see [1] or [2])

$$D_{jk}^{(1)} = \begin{cases} \dfrac{\beta_k/\beta_j}{x_j - x_k}, & j \neq k,\\ -\displaystyle\sum_{i=0,\, i\neq j}^{N} D_{ji}^{(1)}, & j = k, \end{cases} \tag{7}$$

and

$$D_{jk}^{(2)} = \begin{cases} 2D_{jk}^{(1)}\left(D_{jj}^{(1)} - \dfrac{1}{x_j - x_k}\right) & j \neq k,\\ -\displaystyle\sum_{i=0, i\neq j}^{N} D_{ji}^{(2)}, & j = k. \end{cases} \tag{8}$$

A simple proof is given in [6]. In order to alleviate roundoff, formulae (7) and (8) should be used in the calculation of derivatives in the polynomial case as well, see [1].

In the first section, we describe the linear rational collocation method with preassigned poles and recall some useful results on the corresponding interpolation. In section 2, we show that the rational collocation method is equivalent to an associated polynomial collocation method and that it is therefore spectrally accurate if the solution itself has the prescribed poles. Numerical results with the Chebyshev rational and polynomial collocation methods are discussed in the last section.

2. Determination of the barycentric weights

The linear rational collocation method with preassigned poles addressed here consists in choosing the β_k in (2) in order that the denominator has preassigned zeros. Let us write u_N as

$$u_N(x) := \frac{v_N(x)}{d(x)} = \frac{\sum_{k=0}^{N} \tilde{v}_k L_k(x)}{d(x)}, \quad L_k(x) = \frac{w_k/(x-x_k)}{\sum_{i=0}^{n} w_i/(x-x_i)}; \tag{9}$$

v_N is the polynomial of degree at most N interpolating the values $\tilde{u}_k d(x_k)$, $k = 0(1)N$, and the L_k are the Lagrange fundamental polynomials.

In the remainder of this section we recall some results of [5] about the rational interpolant (9). That work addressed the more general problem of computing rational interpolants with, say, ν preassigned poles, that is of finding

$$r = \frac{p}{q} \in \mathcal{R}_{m,n+\nu}, \quad m+n = N, \ \nu \leqslant N-n, \tag{10}$$

such that

$$r(x_k) = \tilde{u}_k, \quad k = 0(1)N. \tag{11}$$

Here we are concerned with the case where all the poles are preassigned, i.e., $n = 0$.

Let us denote the poles to be preassigned by z_j, $j = 1(1)P$, and their respective multiplicities by ν_j ($\nu = \sum_{j=1}^{P} \nu_j \leqslant N$), with all the z_j different from the interpolating points x_k. One therefore has $d(x) = a\prod_{j=1}^{P}(x-z_j)^{\nu_j}$, $a \in \mathbb{C}$. Writing d as the polynomial interpolating itself between the x_k, the corresponding β_k are easily obtained [8] by multiplying the weights w_k of the polynomial interpolant by a multiple of

$$d_k := d(x_k) = a\prod_{j=1}^{P}(x_k - z_j)^{\nu_j}, \quad k = 0(1)N,$$

to get

$$u_N(x) := \frac{\sum_{k=0}^{N}(d_k w_k/(x-x_k))\tilde{u}_k}{\sum_{k=0}^{N} d_k w_k/(x-x_k)}, \tag{12}$$

the barycentric form of the rational interpolant with P preassigned poles (when such an interpolant exists [8], otherwise some or all of the poles are absent). Dividing all the d_k's by $\prod_{j=1}^{P} z_j$, one sees that the polynomial interpolant is the case when all the z_j are at infinity.

The weights $d_k w_k$ $(= \beta_k)$ in (12) do not depend on the interpolated function: the rational interpolation process is linear.

3. Convergence

The results obtained in [7] could be used to prove the convergence of the linear rational collocation method with preassigned poles. A different approach consists in showing that the linear rational collocation method applied to the BVP (1) is equivalent to a polynomial collocation method applied to an associated boundary value problem. One can then apply the results presented in [13] or [22] (for example) to the equivalent associated polynomial collocation method. Before proceeding in this direction, let us recall some facts.

The authors of [17] have studied a rational collocation method applied to the general linear differential equation

$$T[u](x) = \sum_{k=0}^{m} e_k(x)u^{(k)}(x) = f(x), \quad x \in [a,b], \tag{13}$$

with the m linearly independent boundary conditions

$$\sum_{k=0}^{m-1}\bigl(\alpha_{ik}u^{(k)}(a) + \beta_{ik}u^{(k)}(b)\bigr) = 0, \quad \alpha_{i,k}, \beta_{i,k} \in \mathbb{R},\ 1 \leqslant i \leqslant m. \tag{14}$$

They have shown that a rational collocation method with a trial function such as u_N in (3) or (9) is equivalent to a polynomial collocation method applied to an *associated boundary value problem* (ABVP) involving the denominator of the trial rational.

Before stating the main result of [17], we recall some notations. Consider the collocation points x_k on $[a,b]$ with $a = x_0 < x_1 < \cdots < x_N = b$, and let $\mathcal{P}_N$ be the space of polynomials of degree up to N over $[a,b]$. We denote by $\overline{\mathcal{R}}_{N,\nu}$ the set of rational functions in $\mathcal{R}_{N,\nu}$ satisfying the boundary conditions (14), and we set $\overline{\mathcal{P}}_N := \overline{\mathcal{R}}_{N,0}$.

The main result of [17] then is the following.

Theorem 1. Let d be a polynomial of degree ν and $T[u](x) = \sum_{k=0}^{m} e_k(x)u^{(k)}(x)$ be a linear differential operator of order m. Then there exist a finite number of constants α'_{ik}, β'_{ik}, $1 \leqslant i \leqslant m$, such that the collocation matrix on $\overline{\mathcal{R}}_{N,\nu}$ for the problem (13)–(14) is equivalent to the collocation matrix on $\overline{\mathcal{P}}_N$ for the problem

$$T_d[v](x) := \sum_{k=0}^{m} f_k(x)v^{(k)}(x) = f(x)d(x), \tag{15}$$

$$\sum_{k=0}^{m-1} \alpha'_{ik}v^{(k)}(a) + \beta'_{ik}v^{(k)}(b) = 0, \quad 1 \leqslant i \leqslant m, \tag{16}$$

when the same collocation points x_j, $j = 0(1)N$, are used in both BVPs. The coefficients f_k and the constants α'_{ik}, β'_{ik} depend on d and can be computed iteratively.

Indeed, the f_k's can be computed as

$$\begin{aligned} f_{k-1}(x) &= -\frac{d'(x)}{d(x)} k f_k(x) - \frac{d''(x)}{d(x)} \frac{k(k+1)}{2!} f_{k+1}(x) - \cdots \\ &\quad - \frac{d^{\nu}(x)}{d(x)} \frac{k(k+1)\cdots(\nu+k-1)}{k!} f_{k+\nu-1}(x) + e_{k-1}(x), \\ &\quad k = m, m-1, \ldots, 1, \\ f_m(x) &= e_m(x), \qquad f_{m+1}(x) = f_{m+2}(x) = \cdots = f_{m+\nu+1}(x) = 0. \end{aligned}$$

The constants α'_{ik}, β'_{ik} may be computed by iterative formulae as well, see [17].

The previous result clearly shows that, from a theoretical point of view, solving the BVP (13)–(14) with rational collocation is equivalent to applying polynomial collocation to the ABVP (15)–(16).

Corollary 1. Let the solution u of (13)–(14) be meromorphic with poles at $z_1, \ldots, z_P$. Then the linear rational collocation method with trial function (12) converges exponentially toward u, and as fast as the polynomial collocation solution of the ABVP (15)–(16).

Proof. One simply has to transform the problem (13)–(14) into the associated problem (15)–(16) and to apply results of [10,13,22]. □

The idea of transforming the problem into an associated one was also used in [2] for proving the convergence of the rational collocation method for partial differential equations.

4. Numerical examples

In this section we present three numerical examples for the sake of comparing the Chebyshev rational pseudospectral method with preassigned poles with the Chebyshev polynomial pseudospectral method. All our computations where done with Matlab 5.2.1 on a Macintosh G3. We use the same points $x_k := \cos(k\pi/N)$, $k = 0(1)N$, throughout.

The linear systems (4) were solved by Gaussian elimination. The tables display the maximum absolute error E_{abs} at the collocation points.

4.1. Example 1

The first example,

$$\begin{aligned} & u''(x) - u'(x)\left(1 - \frac{1}{x - 0.01}\right) - \frac{u(x)}{(x-0.01)^2} = 0, \\ & u(-1) = -\frac{1}{1.01\mathrm{e}}, \qquad u(0) = -100, \end{aligned}$$

Table 1
Maximum absolute error of the numerical solutions in example 1.

N	Chebyshev collocation	Rational collocation
5	$7.810 \cdot 10^{0}$	$2.180 \cdot 10^{-6}$
10	$2.227 \cdot 10^{0}$	$3.020 \cdot 10^{-14}$
20	$5.703 \cdot 10^{-1}$	$4.400 \cdot 10^{-12}$
40	$1.600 \cdot 10^{-2}$	$1.454 \cdot 10^{-11}$
80	$3.087 \cdot 10^{-6}$	$5.444 \cdot 10^{-11}$

Table 2
Condition number of the matrix **A** of example 1.

N	Chebyshev collocation	Rational collocation
5	$1.557 \cdot 10^{1}$	$1.161 \cdot 10^{1}$
10	$1.844 \cdot 10^{2}$	$1.640 \cdot 10^{2}$
20	$2.320 \cdot 10^{3}$	$2.486 \cdot 10^{3}$
40	$3.415 \cdot 10^{4}$	$3.763 \cdot 10^{4}$
80	$5.448 \cdot 10^{5}$	$5.620 \cdot 10^{5}$

is a slightly modified version of a problem given in [17]. The differential equation is of Fuchsian type and the theory locates a pole at 0.01, see [16, p. 370]. In fact, the exact solution is $u(x) = \mathrm{e}^x/(x - 0.01)$ and it becomes steeper and steeper when approaching the right boundary.

Here, the polynomial d (of degree 1) of theorem 1 is given by $d(x) = x - 0.01$ and the (associated) differential expression $T_d[v]$ by

$$v''(x) - v'(x)\left(1 + \frac{1}{x - 0.01}\right) + \frac{v(x)}{x - 0.01} = 0,$$

$$v(-1) = \frac{1}{\mathrm{e}}, \qquad v(0) = 1.$$

The exact solution is now $v(x) = \mathrm{e}^x$. Since this solution has no singularities in the finite complex plane, the convergence rate is faster than exponential, or super-geometric, as defined in [10]. This very rapid convergence is confirmed in table 1.

In table 1, we display E_{abs} for the rational collocation method with the preassigned pole $z = 0.01$ and compare it to the Chebyshev collocation method. Taking advantage of the knowledge of the location of the pole improves markedly upon the classical Chebyshev collocation method: for 10 points, for example, the absolute error improves by 14 powers of 10.

The error with the rational collocation method increases from $3 \cdot 10^{-14}$ with $N = 10$ to $5 \cdot 10^{-11}$ with $N = 80$. The large condition number of the matrix **A**, as displayed in table 2, is probably responsible for this loss of precision [19, p. 37]. Notice however that the condition number is only marginally more related to the rational error than to the polynomial one (see [4] or [21] for a discussion of this relation for the polynomial case).

Table 3
Maximum absolute error of the numerical solutions in example 2 with $a = 100$, $m = 10$.

N	Chebyshev collocation	Rational collocation
5	$1.188 \cdot 10^{-2}$	$1.174 \cdot 10^{-2}$
10	$2.288 \cdot 10^{1}$	$2.060 \cdot 10^{-1}$
20	$7.657 \cdot 10^{-3}$	$1.637 \cdot 10^{-7}$
40	$8.128 \cdot 10^{-4}$	$3.574 \cdot 10^{-15}$
80	$8.489 \cdot 10^{-6}$	$7.772 \cdot 10^{-15}$

4.2. *Example 2*

Our second example was chosen as

$$u''(x) + \frac{4ax}{1+ax^2}u'(x) + \left(m^2 + \frac{2a}{1+ax^2}\right)u(x) = 0, \quad a > 0,$$
$$u(-1) = -\frac{\sin(m)}{1+a}, \qquad u(1) = \frac{\sin(m)}{1+a},$$

and its solution is

$$u(x) = \frac{\sin(mx)}{1+ax^2}.$$

u has the two poles

$$z_{1,2} = \pm \mathrm{i}\sqrt{\frac{1}{a}},$$

which is not too surprising in view of the differential equation. Since the solution has steep derivatives near 0, the polynomial collocation method will not give good results for small N as the points are clustered around the extremities (-1 and 1). We may expect better results from the rational collocation method with the two preassigned poles.

In table 3, we see that for $a = 100$ and $m = 10$ the linear rational pseudospectral method with the two preassigned poles behaves better than the polynomial method. For $N = 40$, for example, the rational solution provides 11 extra powers of 10. The reader will have noticed that the results of table 3 are worse with $N = 10$ than with $N = 5$. This arises from the fact that the the maximum absolute error E_{abs} is computed at the collocation points only. With 6 points ($N = 5$) the solver is given less information on the singular behaviour of p and q than with 11 points.

4.3. *Example 3*

The third example is a boundary layer problem borrowed from [23],

$$\begin{aligned} &\varepsilon u''(x) + (1+\varepsilon)u'(x) + u(x) = 0, \\ &u(0) = 0, \qquad u(1) = 1. \end{aligned} \tag{17}$$

The exact solution is

$$u(x) = \frac{e^{-x} - e^{-x/\varepsilon}}{e^{-1} - e^{-1/\varepsilon}};$$

for small ε, it has a boundary layer at $x = 0$. Here the differential equation does not provide information about where to locate the poles.

Weideman in [23] has performed a boundary layer analysis to find where to preassign the poles for a rational approximation. A boundary layer analysis consists in finding two approximate solutions, that is an outer solution that is valid in the region where the solution is slowly varying and an inner solution in the boundary layer. For the problem (17), these solutions are given by

$$u_{\text{in}}(x) = e - e^{1-x/\varepsilon}, \qquad u_{\text{out}}(x) = e^{1-x}.$$

Weideman then applies the (5, 5) Padé approximation to the exponential and makes the change of variable $x \leftrightarrow 1 - x/\varepsilon$ to obtain the Padé approximation to u_{in}.

For $\varepsilon = 0.001$ he gives the five poles

$$z_1 \approx -0.0063, \qquad z_{2,3} \approx -0.0057 \pm 0.0035\,\text{i}, \qquad z_{4,5} \approx -0.0036 \pm 0.0071\,\text{i}.$$

For more information on boundary layer analysis, see [3].

We have used these same points as preassigned poles in our method. The maximum abolute error E_{abs} is displayed in table 4, again for the Chebyshev collocation method and the rational method. We see that, for $N = 80$, the latter improves upon the polynomial method by three powers of 10.

Our rational method is obviously a good alternative to other methods when the location of the poles is known or may be guessed at the onset. Compared to the rational method presented in [23] it does not involve any extra computation for finding particular collocation points. (In fact, with Chebyshev points the method of [23] becomes mathematically equivalent to the one suggested here.) However, the specific points used in [23] are superior, as they are spaced more densely at the steep gradient(s) and the additional work to compute them is compensated by the gain in accuracy, see [12] for a more detailed analysis.

Table 4
Maximum absolute error of the numerical solutions in example 3 with $\varepsilon = 0.001$.

N	Chebyshev collocation	Rational collocation
5	$2.132 \cdot 10^{0}$	$5.066 \cdot 10^{0}$
10	$7.375 \cdot 10^{0}$	$2.745 \cdot 10^{-3}$
20	$5.802 \cdot 10^{0}$	$4.451 \cdot 10^{-3}$
40	$3.680 \cdot 10^{-1}$	$4.634 \cdot 10^{-4}$
80	$1.252 \cdot 10^{-3}$	$1.586 \cdot 10^{-6}$

5. Conclusion

In the present work we have presented a linear rational pseudospectral method with preassigned poles. For its implementation, one simply has to alter the polynomial pseudospectral method (based, for example, on Chebyshev points of the second kind) by modifying the weights in the differentiation matrices in accordance with the poles. We have shown that the theoretical convergence results for the classical polynomial pseudospectral method can be used in the rational setting by considering an associated boundary value problem. Finally, we have applied this rational method to three different problems and we have seen that it is often much more efficient than the corresponding polynomial pseudospectral method.

Our way of attaching poles to the polynomial trial function can in principle be used also with nonlinear problems, for which the collocation method is ideally suited (see [14, p. 130]). There, however, determining the precise location of poles could be impossible. One would have to deduce them either from the polynomial solution or by a WKB analysis (see [3, p. 463]), or, better, to successively optimize them as in [9].

Higher-dimensional problems can be tackeled as well in the tensor product case, e.g., when $u(x, y) = \sum_i v_i(x)w_i(y)$. The formulae for two-dimensional rational interpolants with prescribed poles are given in [9]. However, it should not be concealed that the theory of functions of a single complex variable does not generalize straighforwardly to arbitrary functions of several variables.

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