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THE LINEAR RATIONAL PSEUDOSPECTRAL METHOD FOR BOUNDARY VALUE PROBLEMS*

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Abstract.

We consider the version of the pseudospectral method for solving boundary value problems which replaces the differential operator with a matrix constructed from the elementary differentiation matrices whose elements are the derivatives of the Lagrange fundamental polynomials at the collocation points. The iterative solution of the resulting system of equations then requires the recurrent application of that differentiation matrix. Since global polynomial interpolation on the interval only gives useful approximants for points which accumulate in the vicinity of the extremities, the matrix is ill-conditioned. To reduce this drawback, we use Kosloff and Tal-Ezer's suggestion to shift the collocation points closer to equidistant by a conformal map. However, instead of applying their change of variable setting, we extend to stationary equations the linear rational collocation method introduced in former work on partial differential equations. Numerically about as efficient, this does not require any new coding if one starts from an efficient program for the polynomial differentiation matrices.

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Key words: Boundary value problems, collocation, pseudospectral methods, iterative methods.

1 The polynomial and the linear rational collocation methods.

Object of the present work is the numerical solution of linear two-point boundary value problems (BVPs)

$$(1.1)\qquad (Tu)(x) := u''(x) + p(x)u'(x) + q(x)u(x) = f(x), \quad x \in (-1,1),$$
$$u(-1) = u_\ell, \quad u(1) = u_r,$$

by so-called *pseudospectral* (or *spectral collocation) methods.* A classical polynomial version of the latter consists of the following two steps:

1. Replace the solution in (1.1) with the polynomial interpolating between $n+1$ well chosen distinct points (nodes) $x_0, x_1, \ldots, x_n$, written in its Lagrangian form

$$(1.2)\qquad u_n(x) := \sum_{j=0}^{n} \widetilde{u}_j \ell_j(x), \qquad \ell_j(x) := \frac{\prod_{k\neq j}(x - x_k)}{\prod_{k\neq j}(x_j - x_k)}.$$

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If one chooses $\widetilde{u}_0 = u_r$, $\widetilde{u}_n = u_\ell$, the $n-1$ unknowns $\widetilde{u}_j$ for $j = 1, \ldots, n-1$ remain to be determined.

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

$$(Tu_n)(x_i) = f(x_i), \quad i = 1, \ldots, n-1, \tag{1.3}$$

for the remaining $\widetilde{u}_j$'s. If all functions arising in (1.1) are analytic (i.e., holomorphic) then the convergence of u_n toward u as $n \to \infty$ is spectral, i.e., faster than any negative power of n.

In preparation for the introduction of the linear rational collocation method, as presented in [6] for time evolution problems, we rewrite the ℓ_j's as

$$\ell_j(x) = \frac{\lambda_j}{x - x_j} \Big/ \sum_{k=0}^{n} \frac{\lambda_k}{x - x_k}, \quad j = 0, 1, \ldots, n, \tag{1.4}$$
$$\lambda_j := 1 \Big/ \prod_{k \neq j} (x_j - x_k).$$

Then (1.2) becomes the barycentric form [22] of the polynomial u_n,

$$u_n(x) = \sum_{j=0}^{n} \frac{\lambda_j}{x - x_j} \widetilde{u}_j \Big/ \sum_{j=0}^{n} \frac{\lambda_j}{x - x_j}.$$

One of the many advantages of this representation is the fact that common factors in the so-called *weights* λ_j can be cancelled: for instance, simplified weights for Chebyshev points of the second kind $\cos \phi_j$, $\phi_j := j\frac{\pi}{n}$, are given by

$$\lambda_j^* = (-1)^j \delta_j, \qquad \delta_j := \begin{cases} 1/2, & j = 0 \text{ or } j = n, \\ 1, & \text{otherwise.} \end{cases} \tag{1.5}$$

Since polynomial interpolation for arbitrary points is divergent or ill-conditioned, the x_j's cannot be chosen at will. In practice they are projections onto the diameter $[-1, 1]$ of points on the circle that are either equidistant (which yields Chebyshev points) or nearly equidistant (e.g., Legendre points).

It has however been shown in [4] that the points can be conformally moved from their favorable position without significant loss in the precision of approximation if rational is substituted for polynomial interpolation. (On the other hand, numerical experiments seem to show that, in general, direct polynomial interpolation between the shifted points is not very accurate.) In the barycentric setting this simply happens by replacing the weights λ_j in (1.4) with other numbers $[\beta_0, \ldots, \beta_n]^T =: \beta$, still one per node. This means replacing the (linear) polynomial space spanned by the Lagrange fundamental polynomials (1.4) with the linear space $\mathcal{R}^{(\beta)}$ spanned by the fundamental rational functions

$$\ell_j^{(\beta)}(x) := \frac{\beta_j}{x - x_j} \Big/ \sum_{k=0}^{n} \frac{\beta_k}{x - x_k}, \quad j = 0, 1, \ldots, n. \tag{1.6}$$

Let E_ρ, $\rho > 1$, denote the ellipse with foci at ± 1 and with the sum of its axes equal to 2ρ, and let $\mathcal{E}_\rho$ be the interior of E_ρ. The following result holds [4].

THEOREM 1.1. *Let $\mathcal{D}_1$, $\mathcal{D}_2$ be two domains of $\mathbb{C}$ containing $J = [-1, 1]$, respectively I ($\in \mathbb{R}$), let g be a conformal map $\mathcal{D}_1 \to \mathcal{D}_2$ such that $g(J) = I$, and f be a function $\mathcal{D}_2 \to \mathbb{C}$ such that the composition $f \circ g : \mathcal{D}_1 \to \mathbb{C}$ is analytic inside and on E_ρ ($\subset \mathcal{D}_1$). Let $r(x) := \sum_{j=0}^{n} f(x_j)\ell_j^{(\beta)}(x)$, $x = g(y)$, be the rational function with weights* (1.5) *interpolating f between the transformed Chebyshev points $x_j := g(y_j)$. Then, for $x \in [-1, 1]$, $|f(x) - r(x)| = \mathcal{O}(\rho^{-n})$.*

We thus have exponential convergence in n.

REMARK 1.1. A careful study of the proof in [4] shows that, if f is analytic in $g(\mathcal{E}_\sigma)$, $\sigma > \rho$, $\mathcal{E}_\sigma \subset \mathcal{D}_1$, then the error bound

$$|f(z) - r(z)| = \mathcal{O}(\rho^{-n})$$

is valid for $z \in g(\mathcal{E}_\rho) \cup g(E_\rho)$. Indeed, the proof makes merely use of the convergence in $\mathcal{E}_\sigma$ of the sequence of polynomials interpolating between Chebyshev points and this convergence is exponential uniformly on every compactum contained in $\mathcal{E}_\sigma$ (see the proof in [13, p. 174]).

Replacing the polynomial ansatz (1.2) with its rational counterpart

$$u_n(x) := \sum_{j=0}^{n} \widetilde{u}_j \ell_j^{(\beta)}(x), \tag{1.7}$$

i.e., polynomial collocation with its linear rational generalization, does not have any influence on the work needed for solving (1.1). In fact, for every choice of β, (1.3) reads

$$\mathbf{A}\widetilde{\mathbf{u}} = \mathbf{f}, \qquad \mathbf{A} := \mathbf{D}^{(2)} + \mathbf{P}\mathbf{D}^{(1)} + \mathbf{Q}, \tag{1.8}$$

where

$$\begin{aligned}
\widetilde{\mathbf{u}} &:= [\widetilde{u}_1, \widetilde{u}_2, \ldots, \widetilde{u}_{n-1}]^T, \\
\mathbf{D}^{(1)} &= \big(D_{ij}^{(1)}\big), \qquad D_{ij}^{(1)} := \ell_j^{(\beta)\prime}(x_i), \\
\mathbf{D}^{(2)} &= \big(D_{ij}^{(2)}\big), \qquad D_{ij}^{(2)} := \ell_j^{(\beta)\prime\prime}(x_i), \\
\mathbf{P} &:= \operatorname{diag}\big(p(x_i)\big), \qquad \mathbf{Q} := \operatorname{diag}\big(q(x_i)\big), \\
\mathbf{f} &:= [f(x_i) - u_r\big(\ell_0^{(\beta)\prime\prime}(x_i) + p(x_i)\ell_0^{(\beta)\prime}(x_i)\big) - u_\ell\big(\ell_n^{(\beta)\prime\prime}(x_i) + p(x_i)\ell_n^{(\beta)\prime}(x_i)\big)]^T, \\
&\qquad i,\ j = 1, \ldots, n-1.
\end{aligned}$$

The differentiation matrices $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$ can be given by the formulae [5, 7]

$$D_{ij}^{(1)} = \begin{cases} \dfrac{\beta_j/\beta_i}{x_i - x_j}, & i \neq j, \\ -\displaystyle\sum_{k \neq i} D_{ik}^{(1)}, & i = j, \end{cases} \qquad D_{ij}^{(2)} = \begin{cases} 2D_{ij}^{(1)}\Big(D_{ii}^{(1)} - \dfrac{1}{x_i - x_j}\Big), & i \neq j, \\ -\displaystyle\sum_{k \neq i} D_{ik}^{(2)}, & i = j. \end{cases}$$

Although more expensive to evaluate than specific ones, the same formulae for the diagonal elements should be used also in the polynomial case [5]. Then a

change of points such as those considered in the present work does not require any modification in the matrix subprograms.

In the iterative methods used for the efficient solution of (1.8) the matrix $\mathbf{A}$, and thus explicitly or implicitly $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$, are repetitively applied to vectors approximating $\widetilde{\mathbf{u}}$. But for points favorable for interpolation, the operators $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$ are ill-conditioned [24, 5], severely for large n. We will demonstrate in the present work that conformal point shifts can be interesting for improving upon the condition of the multiplication by $\mathbf{A}$ without loss in precision.

2 Spectral convergence with point shifts.

We now discuss the solution of the BVP (1.1) with the collocation method (1.3) for the linear rational interpolant $u_n(x) = \sum_{j=0}^{n} \widetilde{u}_j \ell_j^{(\beta)}(x)$, with $\ell_j^{(\beta)}$ as in (1.6). The points will be shifted Chebyshev points and the weights β the Chebyshev weights of the second kind (1.5). Let $y_j = \cos\phi_j$, $\phi_j := j\frac{\pi}{n}$, be the Chebyshev points of the second kind. We consider a conformal map g of the ellipse $\mathcal{E}_\rho$ containing the y-interval $J := [-1, 1]$ of the y_j's onto the domain $\mathcal{F}_\rho := g(\mathcal{E}_\rho)$ containing the interval $I := [-1, 1]$ such that $g(J) = I$. This defines a new set of points $x_j := g(y_j)$. g will be chosen in such a way that our collocation points x_j are closer to equidistant than the y_j. In practical computations we will use, as in [6], a map suggested by Kosloff and Tal-Ezer [17],

$$g(y) = \frac{\arcsin(\alpha y)}{\arcsin\alpha}, \qquad 0 < \alpha < 1. \tag{2.1}$$

In the limit $\alpha \to 0$, $x_i = y_i$; as $\alpha \to 1$, the x_i become equidistant.

Kosloff and Tal-Ezer have used such point shifts for improving the stability of the numerical methods which solve in time the spatially discretized time evolution partial differential equations. Here we will use them with the iterative solution of the collocation equations (1.3), resp. (1.8). In both cases the point shift improves upon the condition of the differentiation process.

Before we consider this iterative procedure, we will discuss why we think the exponential convergence of u_n toward u is maintained while shifting points.

The set $\mathcal{A}$ of all functions h that are analytic (holomorphic) in $\mathcal{F}_\rho$ and continuous in $\mathcal{F}_\rho \cup F_\rho$, $F_\rho := g(E_\rho)$, with the norm $|h| := \max_{z\in F_\rho} |h(z)|$ is a (complex) Banach space. We will use the Sobolev idea pervasive in the context of differential equations and consider our problem in the Banach space

$$\mathcal{B}^{(\rho)} := \{v : \ v,\ v', v'' \text{ and } v''' \in \mathcal{A},\ \|v\| := |v| + |v'| + |v''| < \infty\}.$$

Moreover, we will assume that $p \in \mathcal{A}$, $q \in \mathcal{A}$ and $q \neq 0$ ($q < 0$ is a property that guarantees the existence of a unique solution of (1.1); see [15]). Then we can divide equation (1.1) by q, write it in functional form as

$$u + \frac{p}{q}u' + \frac{1}{q}u'' = \frac{f}{q}$$

and consider the operator L that to every $v \in \mathcal{B}^{(\rho)}$ associates the function $Lv := \frac{p}{q}v' + \frac{1}{q}v'' \in \mathcal{B}^{(\rho)}$. (1.1) may be written as

$$(I + L)u = h, \qquad h := f/q. \tag{2.2}$$

To warrant compliance with the boundary values while keeping the space linear, it will as usual be assumed that $u(-1) = u(1) = 0$, which can be attained by subtracting a known function from u and changing f accordingly. (There is no need for this in practical computations.) We therefore consider the Banach space

$$\mathcal{B}^0 := \{v \in \mathcal{B}^{(\rho)}:\ v(-1) = v(1) = 0\}.$$

The linear operator $I+L : \mathcal{B}^0 \to (I+L)\ \mathcal{B}^0 \subset \mathcal{A}$ is obviously bounded, with $\|I+L\| \leq 1 + \|L\|$ and $\|L\| \leq \left|\frac{p}{q}\right| + \left|\frac{1}{q}\right|$. We assume that (2.2) has a unique solution for every h (see, e.g., [15] or [1] for conditions that guarantee this); since $(I + L)\ \mathcal{B}^0$ is a Banach space, this implies by the bounded inverse theorem ([18, p. 286]) that $I+L$ possesses a bounded inverse $(I + L)^{-1}$.

No simple general theory of collocation methods for boundary problems exists, this in contrast with the situation in the numerical solution of Fredholm integral equations, for example, where they are a special case of projection methods [3]—see, however, [21]. We will use the theory of projection methods to motivate that, for a whole class of problems, the linear rational method with shifted Chebyshev points is (exponentially) convergent.

Beside the underlying Banach space $\mathcal{B}$ (here $\mathcal{B}^0$), such methods require a subspace $\mathcal{B}_n$ of finite dimension (which can be seen as an element of an infinite sequence $\mathcal{B}_1,\ \mathcal{B}_2, \ldots$ of such spaces) and a corresponding (sequence of) bounded projection operator(s) $P_n : \mathcal{B} \to \mathcal{B}_n$. In the collocation case, $\mathcal{B}_n$ is taken as a subspace spanned by some elements $\{\phi_j\}$ of $\mathcal{B}$, here $\{\ell_j^{(\beta)}\}_{j=1}^{n-1}$, with

$$\det\left(\phi_j(x_i)\right) = \det\left(\ell_j^{(\beta)}(x_i)\right)_{i,j=1}^{n-1} \neq 0 \tag{2.3}$$

(the dimension is $n-1$ since $\widetilde{u}_0 = \widetilde{u}_n = 0$). The method then consists in inserting u_n of (1.7) into (2.2) to get $(I + L)u_n = h$, projecting this equation into $\mathcal{B}_n$ to get

$$P_n(I + L)u_n = (I + P_nL)u_n = P_nh \tag{2.4}$$

and using the following general theorem on projection methods.

THEOREM 2.1. *Let $\mathcal{B}$ be a Banach space, $\mathcal{B}_n$ a subspace of finite dimension, P_n a bounded projection operator $\mathcal{B} \to \mathcal{B}_n$. Moreover, let $(I + L)^{-1}$ exist and be bounded on the range $\mathcal{R}(I + L)$ and let $\|L - P_nL\| < \frac{1}{\|(I+L)^{-1}\|}$. Then $(I + P_nL)^{-1}$ exists on $\mathcal{R}(I + L)$ and*

$$\|(I + P_nL)^{-1}\| \leq \frac{\|(I + L)^{-1}\|}{1 - \|(I + L)^{-1}\| \cdot \|L - P_nL\|}.$$

Moreover, the distance from the solution u_n of (2.4) to the solution u of (1.1) is bounded by

$$\|u_n - u\| \leq \|(I + P_nL)^{-1}\| \cdot \|u - P_nu\|. \tag{2.5}$$

PROOF. [2, p. 51]. □

The relevance of this theorem in the framework of the collocation method (1.3) is given by the following result.

THEOREM 2.2. *Let* $-1 \equiv x_0, x_1, \ldots, x_n \equiv 1$ *be different points of* $[-1, 1]$, *let* $\{\ell_j^{(\beta)}\}_{j=1}^{n-1}$ *be defined as in* (1.6) *with* $\beta_j \neq 0 \ \forall\ j$, *let*

$$\mathcal{B}_n := \operatorname{span}\{\ell_j^{(\beta)}\}, \quad P_n :\ v \to \sum_{j=1}^{n-1} v(x_j)\ell_j^{(\beta)}(x)$$

be the projection of $\mathcal{B}^0$ *onto* $\mathcal{B}_n$ *and let our collocation method be defined by* (1.3) *with* $\ell_j^{(\beta)}$ *in lieu of* ℓ_j. *Then the latter is a projection method to which Theorem* 2.1 *may be applied.*

PROOF. By definition of $\ell_j^{(\beta)}$ and with $\beta_j \neq 0$, all j, one has $\ell_j^{(\beta)}(x_i) = \delta_{ij}$, the matrix of such quantities is the identity matrix and condition (2.3) is satisfied. The proof of the result is then identical with that in [3, pp. 51–52]. □

Theorems 1.1 and 2.1 help us to explain the (exponential) convergence of the linear rational collocation method in some cases.

First, we conjecture that $P_n v \to v$ for all $v \in \mathcal{B}^{(\rho)}$. Indeed, one has pointwise convergence in $\mathcal{E}_\rho$ of the sequence of the polynomials interpolating v between Chebyshev points (see [13] p. 28). We conjecture that convergence holds on the boundary also. The reason is the fact that the Taylor series of a function f analytic inside the open unit disk and continuous together with its derivative in the closed disk converges also on the unit circle. (In fact, Dini continuity is sufficient for this.) Indeed, if the Taylor coefficients of f are denoted with a_k and the Fourier coefficients of the L_2 boundary function $f(e^{i\phi})$ are denoted with c_k, one has $c_k = a_k$, $k \geq 0$ and $c_k = 0$, $k < 0$ [12, p. 38]. The Fourier coefficients of $\frac{d}{d\phi} f(e^{i\phi})$ are ika_k and must go to zero by the lemma of Riemann-Lebesgue. But then by Tauber's theorem [19, Vol. I, p. 402] the Taylor series of f must converge on the boundary. On the other hand, interpolating polynomials are just a slight generalization of Taylor polynomials [19, Vol. II, p. 70]. And by the remark following Theorem 1.1 this convergence on the boundary will correspondingly hold on $\mathcal{F}_\rho$ for our rational interpolant (1.7).

Second, if our conjecture is true and since we assume the existence of three continuous derivatives for every $v \in \mathcal{B}^{(\rho)}$, we have $\|v - P_n v\| \to 0$, from which it follows that the sequence $\{I - P_n\}$ is strongly operator convergent [18, p. 264] toward the zero-operator and therefore that $\{\|I - P_n\|\}$ is bounded [ibid. p. 267]. Thus, if $\|L\|$ is small enough, all the hypotheses of Theorem 2.1 are satisfied, $(I + P_n L)^{-1}$ exists and the solution of (1.3) with the basis functions $\ell_j^{(\beta)}$ replacing ℓ_j satisfies (2.5).

Third, if the solution u not only belongs to $\mathcal{B}^{(\rho)}$, but is also analytic on F_ρ, then $|u - P_n u| \to 0$ exponentially, uniformly on every compactum in $\mathcal{F}_\rho \cup F_\rho$, and by Weierstrass' theorem [19, Vol. I, p. 333] the same holds true for the first two derivatives. Then $\|u - P_n u\| \to 0$ exponentially too and by (2.5) the same is true for $\|u_n - u\|$ and $|u_n - u|$.

The same line of reasoning could work also if in the equation the main part is u'', and $Lu := pu' + qu$ is significantly smaller. (If one would then set u'' instead of u

as the unknown rational interpolant, then a rational spectral integration method in the spirit of Greengard [14] would result—see also [26].)

3 Iterative solution of the discretized equations.

In global (pseudo)spectral methods like those considered here, the matrix $\mathbf{A}$ of system (1.8) is full. Whereas for small n classical Gaussian elimination is usually appropriate for its solution, as n becomes larger one must resort to iterative methods for a reasonable computational effort. A vast palet of such methods is available. A simple classical example is *Richardson iteration*

$$\mathbf{u}^{k+1} = \mathbf{u}^k - \gamma(\mathbf{A}\mathbf{u}^k - \mathbf{f}) \tag{3.1}$$

and its variations. Here we will use the *preconditioned minimal residual Richardson method* (MRR), whose efficiency in the context of spectral methods has been demonstrated in [10]. However, we modify it by minimizing the preconditioned residual instead of the residual itself. Possibly first used with spectral methods in [8], it has proved more efficient than classical MRR. If one denotes the preconditioner with $\mathbf{A}_{ap}$, the set of formulae for computing the new approximation $\mathbf{u}^{k+1}$ can be written as follows:

$$\begin{aligned}
\mathbf{r}^k &= \begin{cases} \mathbf{A}_{ap}^{-1}(\mathbf{A}\mathbf{u}^0 - \mathbf{f}), & k = 0, \\ \mathbf{r}^{k-1} - \gamma^{k-1}\mathbf{z}^{k-1}, & k \geq 1, \end{cases} \\
\mathbf{z}^k &= \mathbf{A}_{ap}^{-1}\mathbf{A}\mathbf{r}^k, \\
\gamma^k &= \frac{\left(\mathbf{r}^k, \mathbf{z}^k\right)}{\left(\mathbf{z}^k, \mathbf{z}^k\right)}, \\
\mathbf{u}^{k+1} &= \mathbf{u}^k - \gamma^k\mathbf{r}^k.
\end{aligned}$$

Most other methods, at least among those requiring only the application of $\mathbf{A}$—and not of $\mathbf{A}^T$—could be used as well. However, our purpose here is not the study of the influence of point shifts upon a particular method, but the improvement we think such shifts bring to most if not all methods.

Which preconditioner to use? In the context of spectral methods, S. Orszag's idea of using as $\mathbf{A}_{ap}$ a classical finite difference (FD) approximations to the differentiation operator [20] has become standard. Here we will take the one in which the derivatives are replaced with those of interpolating polynomials of degree 2 [22, p. 113] for unequally spaced points. Such preconditioners have been theoretically studied by Kim and Parter [16]. Finite element (FE) preconditioners have later been suggested [11]; we have however not tried them since the same order of approximation is attained by FD-preconditioners, and again because the effects we want to demonstrate should take place with every choice of $\mathbf{A}_{ap}$.

4 Influence of point shifts upon the discretized operators.

Iterative methods of the form $\mathbf{z}^{k+1} = \mathbf{F}\mathbf{z}^k$ are theoretically governed by the spectrum $S(\mathbf{F})$ of the matrix $\mathbf{F}$: to guarantee convergence of the iteration for

every starting vector $\mathbf{z}^0$, all eigenvalues of $\mathbf{F}$ should lie within the unit disk about the origin. In practice, however, the ill-conditioning of the multiplication by $\mathbf{F}$ must be taken into account and, for that purpose, the *ϵ-pseudospectrum* [25]

$$PS(\mathbf{F}) := \bigcup_{\|\mathbf{E}\| < \epsilon} S(\mathbf{F} + \mathbf{E})$$

of $\mathbf{F}$ is more relevant. If $\mathbf{F}$ is nearly normal, $PS(\mathbf{F})$ is not significantly larger than $S(\mathbf{F})$ and consideration of the latter is adequate. For highly nonnormal matrices such as $\mathbf{A}$, on the other hand, $PS(\mathbf{A})$ expands very rapidly about $S(\mathbf{A})$ as ϵ increases. (Somewhat surprisingly, for Gaussian elimination the severe ill-conditioning of $\mathbf{A}$ does not have any significant impact on the quality of the solution [8, 23]; solving a system of equations is mathematically equivalent to applying the inverse matrix, here a well-conditioned integration operator.)

The reason for the improvement on the condition of $\mathbf{A}$ induced by point shifts is the fact that they reduce the magnitude of the expansion (examples of such dramatic reductions of the size of pseudospectra seem to have first been published in [6]). But here the preconditioner radically changes the picture. In Figure 4.1 (left) we give the 10^{-3}-pseudospectrum of $\mathbf{F}^{(k)} := \mathbf{I} - \gamma_k \mathbf{A}_{ap}^{-1}\mathbf{A}$ for polynomial collocation in Example 2 of Section 5, with $\eta = 1{,}000$, $n = 160$ (see Table 5.2), $k = 20$ (with $\mathbf{u}^0$ given by the line between the boundary points). In sharp contrast with the pseudospectrum of $\mathbf{A}$, $PS(\mathbf{F}^{(k)})$ does almost not depart from $S(\mathbf{F}^{(k)})$: the preconditioner practically annihilates the ill-conditioning! Considering spectra is therefore sufficient here, and Figure 4.1 (right) documents the decrease of $S(\mathbf{F}^{(k)})$ as α increases from 0 (circles) to 0.99 (crosses).

To confirm the extreme efficiency of the preconditioner, we have computed for several examples of Table 5.2 the maximal element (in absolute value) of the difference between the differentiation matrices with and without point shifts, for $\mathbf{A}$ and for the preconditioned $\mathbf{A}_{ap}^{-1}\mathbf{A}$. The results are given in Table 4.1.

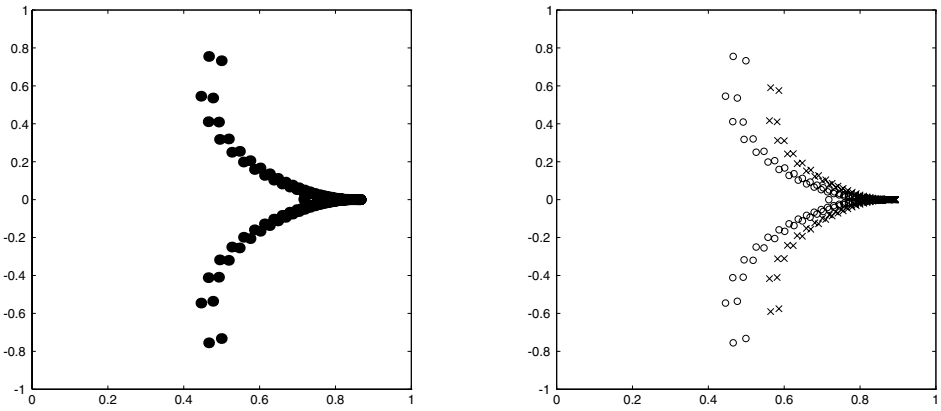

Figure 4.1: Displacement of the spectrum induced by a point shift.

Table 4.1: Influence of the point shifts on the differential operators.

η	n	Change in $\mathbf{A}$	Change in $\mathbf{A}_{ap}^{-1}\mathbf{A}$
1	10	3.72e2	4.07e − 1
1	20	6.52e3	3.12e − 1
10	40	1.08e5	1.29e − 1
100	80	1.75e6	1.61e − 1
1,000	160	2.87e7	6.12e − 1
10,000	320	4.84e8	1.78e0
10,000	640	7.25e9	8.81e − 1
100,000	1280	1.20e11	1.67e0

5 Numerical examples.

For the sake of comparison, we have tested the rational collocation method on the same four examples as in [8] and [9]. Here we merely comment on two problems. Graphs of the solutions can be found in the works just mentioned.

In all examples our interpolation/collocation points have been Chebyshev points of the second kind, shifted by means of the application (2.1) for different α's. The norm of the error has been approximated by considering its values at the 1000 equally spaced points $\widehat{x}_\ell = -\frac{5}{4} + \frac{\ell-1}{999}\frac{10}{4}$, $\ell = 1(1)1000$, on the interval $[-5/4, 5/4]$ and computing the maximal absolute value at those $\widehat{x}_\ell$ lying in $[-1, 1]$. These points depend neither on n nor on α. The iteration process has been performed until the error norm came to lie below the tolerance $n \cdot 10^{-16}$ or until the number of iterations surpassed 2000. (in fact, $n/3$ should be the barrier, In the tables, an error given as 0.0 means that it was $< n \cdot 10^{-16}$. The computations were performed in FORTRAN77 on a DECalpha3000 workstation.

Example 5.1. Our first problem reads

$$u''(x) + au'(x) + bu(x) = -ab\cos(bx)e^{-ax},$$
$$u(0) = 0, \qquad u(1) = \sin b e^{-a}$$

and its solution is given by $u(x) = \sin(bx)e^{-ax}$, where a and b are two positive parameters. b controls the frequency of the oscillations: the higher b, the larger the number of oscillations, and the steeper the function in each of the latters. The change of variable $x = (t + 1)/2$ should be made for the problem to take place in the interval $[-1, 1]$ instead of $[0, 1]$.

In Table 5.1 we give the numbers obtained with $a = 5$, $b = 100$ and 200 and increasing α's (recall that $\alpha = 0$ corresponds to the classical polynomial Chebyshev method). In the starred example, the error $5.46 \cdot 10^{-4}$ was attained after 25 iterations, the difference between consecutive iterates is about $1.97 \cdot 10^{-8}$.

The number of iterations is relatively small with pseudospectral methods, as compared with finite difference or finite element methods; this may be attributed to the analyticity of the arising functions which makes for a good approximation to the solution from the given information. Note also that in principle the quality of

the latter decreases as α increases. Indeed, to every function on the interval there corresponds via the transformation $\phi = \arccos x$ a function on the circle [8]. And the quality of the information on the circle is decisive for that of the approximation. With $\alpha = 0$ the information taken from the problem is at equidistant points on the circle, which is best in the absence of other knowledge. Having α grow means departing from this optimum.

Table 5.1: Reduction of the number of iterations for increasing α in Example 1.

α	$b = 100,\ n = 450$		$b = 200,\ n = 950$	
	Error	# iterations	Error	# iterations
0.0	3.77e − 13	96	5.46e − 4	$> 2000^*$
0.9	7.46e − 14	26	3.97e − 13	30
0.99	1.49e − 13	21	2.31e − 13	21
0.999	1.42e − 12	22	1.60e − 13	19
0.9999	9.41e − 7	23	9.06e − 10	24

Table 5.2: Effect of a point shift on the approximation error and on the number of iterations in Example 2.

η	n	$\alpha = 0.0$		$\alpha = 0.99$	
		Error	# iter.	Error	# iter.
1	10	1.22e − 6	24	2.82e − 3	24
1	20	0.0	16	2.02e − 4	28
10	40	0.0	11	4.96e − 6	26
100	80	0.0	20	1.35e − 8	31
1,000	160	3.69e − 8	134	1.65e − 13	89
10,000	320	1.66e − 4	581	3.34e − 7	434
10,000	640	1.03e − 11	308	1.65e − 12	223
100,000	1280	4.96e − 6	1596	3.53e − 10	1080

Example 5.2. In contrast with the usual case just described, it sometimes happens that the point shift not only speeds up the convergence of the iteration but, more importantly, improves upon the precision of the approximate solution for a given n. This is especially the case when the most difficult part of the solution to be approximated lies far from the extremities of the interval, since the point shift brings the collocation points closer to the center. A good example, to which though the theory of Section 2 does not apply, is the following problem involving a parameter which makes for a large slope in the center:

$$u''(x) + \eta x u'(x) = -\pi^2 \cos(\pi x) - \eta \pi x \sin(\pi x), \quad u(-1) = -2, \quad u(1) = 0.$$

The solution

$$u(x) = \cos \pi x + \frac{\operatorname{erf}(\delta x)}{\operatorname{erf}(\delta)}, \quad \delta = \sqrt{0.5\eta},$$

becomes steeper and steeper at zero as η grows larger.

Table 5.2 displays the said improvement in both the precision and the number of iterations as n is large enough for the main difficulty of the solution to lie inside the interval ($\eta \geq 1000$); the gain is about 1/3. For the easier problems, no gain is recorded, for the same reason of quality of information explained above. In Table 5.3 we give the change in precision and the number of iterations for fixed n and increasing α with two pairs of η and n. They show again that an improvement of one third may be obtained without significant loss in precision.

Table 5.3: Reduction of the number of iterations for increasing α in Example 2.

α	$\eta = 10^3,\ n = 400$		$\eta = 10^4,\ n = 1000$	
	Error	# iterations	Error	# iterations
0.0	6.72e − 14	15	0.0	155
0.9	6.72e − 14	12	0.0	124
0.99	1.04e − 13	10	0.0	109
0.999	2.27e − 12	34	0.0	91
0.9999	4.46e − 7	66	5.09e − 11	217

Our examples demonstrate that, if difficulties arise with the convergence of the iteration, one may just try adding three lines of code for a better positioning of the interpolation points!

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