Approximation on disjoint intervals and its application to matrix preconditioning

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Abstract
A polynomial preconditioner to an invertible matrix can be constructed from the (near) best approximation of the function $1/x$. We use the knowledge that the eigenvalues of the matrix are located in the union of two disjoint regions.

Estimates are presented that show that the method can beat the computational complexity of full inversion by one order of magnitude in the size of the matrix. It shows that the error that measures the fit between the polynomial approximation and the function $1/x$ depends on the order of the polynomial, rather than on the matrix size.

An algorithm, based on the strategy, is implemented and tested on a number of concrete cases. It is found that the algorithm is numerically stable, very accurate, and does not require a very precise delineation of the boundaries between the two disjoint intervals, so long as the guess as to where this boundary exists does not intercept either eigenvalue region.

1 Introduction

Let $A$ be an invertible matrix whose spectrum is such that we can clearly enclose its two distinct clusters of eigenvalues by non-joining delineating curves. In what follows we will focus on matrices that are symmetric positive definite, hence, with real eigenvalues. However, the results presented here generalize to the case of normal matrix and thus to a complex spectrum. For the sake of simplicity we will assume that the clusters of eigenvalues are contained in $[-b,-a] \cup [a,b]$, where $0 < a < b$. The intervals can be made sufficiently large so as to contain the eigenvalue clusters and be symmetric about zero, possibly with the requirement of a shift.

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For such a matrix we present here the construction and the practical implementation of an algorithm that computes a preconditioner $B$ of the form $P_n(A)$, where $P_n$ is a polynomial of (low) degree $n$. The manner in which this is obtained is by approximating the function $1/x$.

The preconditioner, once found can be used to accelerate the task of finding a solution of the linear algebraic problem $Ax = b$ by iterative means (pertinent to our approximation strategy, the reader is referred to [2] and [11]).

It should be said from the outset that the efficient solution of linear algebraic problems involving symmetric positive definite (indeed, more generally normal) matrices has had a long research history and methods such as multigrid, conjugate gradient, and multipole are well established optimal or near optimal methods. We are not proposing a solution strategy that will be in the same league as the most efficient methods available. Our focus is on approximation theory, the present contribution a necessary first step in understanding how to approximate $1/z$ when $A$ is normal and has a spectrum composed of distinct islands of eigenvalues. In our closing comments we will discuss how the present work relates to the more general one.

Two results are fundamental to the preconditioner construction. The following are well known, and are presented here for the more general case of normal matrices with complex spectra (see for example [4], [6], [7] and [12]):

**Theorem 1.1.** Let $\Gamma$ be a (closed) curve enclosing the eigenvalues $S_P(A)$ of the normal matrix $A$. Let $f(z)$ be analytic on and inside $\Gamma$, $\Gamma$ encloses $S_P(A)$ and let $P_n(z)$ be a polynomial approximating (uniformly) $f(z)$ on $\Gamma$.

Then

$$
\|f(A) - P_n(A)\| = \sup_{z \in S_P(A)} |f(z) - P_n(z)| \\
\leq \sup_{z \in \Gamma} |f(z) - P_n(z)|.
$$

*Here $\|\|$ stands for the matrix 2-norm.*

The equality above is consequence of the spectral theorem for normal operators. The inequality is a consequence of the maximum principle for analytic functions. We now specialize the above result in the context where $f(z) = \frac{1}{z}$.

**Corollary 1.1.** Let $f(z) = \frac{1}{z}$ and let $P_n(z)$ be a polynomial approximating (uniformly) $f(z)$ on $\Gamma$. (0 $\in$ Ext($\Gamma$).) Then, if $A$ is normal,

$$
\|A^{-1} - P_n(A)\| = \sup_{z \in S_p(A)} \left| \frac{1}{z} - P_n(z) \right| \leq \sup_{z \in \Gamma} \left| \frac{1}{z} - P_n(z) \right|.
$$

(1.1)
2 Construction of the Polynomial of (near) Best Approximation to $\frac{1}{x}$ on $[-b, -a] \cup [a, b]$

The approximation theory result on which our procedure is based is the following theorem due to Bernstein [1], [12].

**Theorem 2.1.** Let $|\alpha| > 1$ and let $P_n(x)$ be the polynomial of best approximation of $\frac{1}{x-\alpha}$ on $[-1, 1]$. Then there exist constants $C_1$, $C_2$ such that

$$C_1 \left( |\alpha| - \sqrt{\alpha^2 - 1} \right)^n \leq \left\| P_n(x) - \frac{1}{x - \alpha} \right\| \leq C_2 \left( |\alpha| - \sqrt{\alpha^2 - 1} \right)^n.$$

**Corollary 2.1.** Let $0 < a < b$ and let $P_n(x)$ be the polynomial of best approximation of $\frac{1}{x}$ on $[a, b]$. Then there exist constants $C_1$, $C_2$ such that

$$C_1 \left( \frac{\sqrt{b} - \sqrt{a}}{\sqrt{b} + \sqrt{a}} \right)^n \leq \left\| P_n(x) - \frac{1}{x} \right\| \leq C_2 \left( \frac{\sqrt{b} - \sqrt{a}}{\sqrt{b} + \sqrt{a}} \right)^n.$$

**Proof.** Consider the map $\gamma(x) := \frac{-b}{b - a} - \frac{b + a}{b - a}$ that transforms linearly $[a, b]$ into $[-1, 1]$. The singularity of the transformed function $\frac{1}{(b - a)x + b + a}$, $x \in [-1, 1]$, is now located at $\alpha = \gamma(0) = -\frac{b + a}{b - a}$ so that $|\alpha| - \sqrt{\alpha^2 - 1} = \frac{\sqrt{b} - \sqrt{a}}{\sqrt{b} + \sqrt{a}}$. The proof is now completed by noticing that if $Q_n(x)$ is a polynomial of degree $n$ so is $Q_n(\gamma(x))$. □

We are now ready to construct our polynomials by following the steps below.

**Step 1** Approximate $\frac{1}{x}$ on $[a^2, b^2]$ by $P_n(x)$.

**Step 2** Then $P_n(x^2)$ approximates $\frac{1}{x}$ on $[a, b]$.

**Step 3** Hence $xP_n(x^2)$ approximates $\frac{1}{x}$ on $[a, b]$.

**Step 4** But $xP_n(x^2)$ is an odd polynomial. Hence, because $\frac{1}{x}$ is an odd function, $xP_n(x^2)$ approximates $\frac{1}{x}$ on $[-b, -a] \cup [a, b]$.

The reader may wish to consult [3] for qualitative results about the possibility of such approximation.

The above procedure guarantees only existence of an algorithm to build a polynomial approximating $\frac{1}{x}$. However we wish to build the (near) best approximating polynomial. The method that we will use to build numerically these polynomials is based on the following theorem of Dini-Lipschitz (See [1] and [6].)

**Theorem 2.2.** Let $f(x)$ be a smooth function defined on $[-1, 1]$ and let $E_n(f)$ denote the error between $f(x)$ and the polynomial of degree $n$ of best uniform approximation. Expand $f(x)$ in its Fourier-Chebyshev series, that is to say

$$f(x) = \sum_{n=0}^{\infty} a_n T_n(x)$$

3
where \( T_n(x) \) are the Chebyshev polynomials and

\[
a_n = \alpha_n \int_0^\pi f(\cos(\theta)) \cos(n\theta) d\theta
\]

\( \alpha_n = 1/\pi \) if \( n = 0 \), \( \alpha_n = 2/\pi \) if \( n \geq 1 \). Then

\[
\left\| f(x) - \sum_{k=0}^{n} a_k T_k(x) \right\| = \left\| \sum_{k=n+1}^{\infty} a_k T_k(x) \right\| \leq c \log(n) E_n(f)
\]

In other words, this theorem tells us that the weighted least square approximation, with weight \( 1/\sqrt{1-x^2} \), is almost the best uniform approximation.

Now we have to adapt this theorem to the setting of two intervals. The key will be Corollary 2.1 together with Steps 1 – 4 of the last section.

**Steps 1 and 2.**
We first transform the interval \([-1, 1]\) into the interval \([a^2, b^2]\) by

\[
x \mapsto \frac{1}{2}((b^2 - a^2)x + b^2 + a^2).
\]

The function \( \frac{1}{x} \) becomes now

\[
\frac{1}{\text{frac}12((b^2 - a^2)x + b^2 + a^2)}.
\]

Its Fourier-Chebyshev coefficients are consequently

\[
\alpha_n = \frac{2}{\pi} \int_0^\pi \frac{\cos(n\theta)}{\frac{1}{2}((b^2 - a^2)\cos(\theta) + b^2 + a^2)} d\theta, \quad n \geq 1,
\]

\[
\alpha_0 = \frac{1}{\pi} \int_0^\pi \frac{1}{\frac{1}{2}((b^2 - a^2)\cos(\theta) + b^2 + a^2)} d\theta.
\]

**Steps 3 and 4.**
We now consider

\[
\sum_{k=0}^{n} a_k T_k(x)
\]

where \( T_k(x) \) are the Chebyshev polynomials and go back to the intervals \([-b, -a] \cup [a, b]\) with the mapping

\[
x \mapsto \frac{2x^2}{b^2 - a^2} - \frac{b^2 + a^2}{b^2 - a^2}
\]

to obtain

\[
\sum_{k=0}^{n} a_k T_k \left( \frac{2x^2}{b^2 - a^2} - \frac{b^2 + a^2}{b^2 - a^2} \right).
\]
Hence the required polynomial is

\[ x \sum_{k=0}^{n} a_k T_k \left( \frac{2x^2}{b^2 - a^2} - \frac{b^2 + a^2}{b^2 - a^2} \right). \]  

(2.4)

We remark that as \( x \in [-b, -a] \cup [a, b] \), \( \frac{2x^2}{b^2 - a^2} - \frac{b^2 + a^2}{b^2 - a^2} \in [-1, 1] \). In Figure 2.1 we show the form of the polynomial on two symmetric intervals with \( a = 0.4 \) and \( b = 0.8 \). Of importance is to note that the function grows extremely fast outside of the regions which are occupied by eigenvalues.

![Figure 2.1: \( T_4 \left( \frac{2x^2}{b^2 - a^2} - \frac{b^2 + a^2}{b^2 - a^2} \right) \) for \( a = 0.4 \) and \( b = 0.8 \).](image)

Let us now summarize the result on which our algorithm will be based. We remark that (2.4) above is the translation, in the present setting, of Step 4 of the last section.

**Theorem 2.3.** Let \( f(x) = \frac{1}{x}, \ x \in [-b, -a] \cup [a, b] \). Then the polynomial of near best uniform approximation to \( \frac{1}{x} \) of degree \( 2n + 1 \) on \( [-b, -a] \cup [a, b] \) is given by

\[
P_{2n+1}(x) = x \sum_{k=0}^{n} \frac{2}{\pi} \frac{\cos(k\theta)}{\sqrt{\left(\frac{b}{b^2 - a^2}\right)\cos(\theta) + b^2 + a^2}} d\theta \times \left( T_k \left( \frac{2x^2}{b^2 - a^2} - \frac{b^2 + a^2}{b^2 - a^2} \right) \right),
\]

(2.5)

where \( T_k(u) = \cos(k \arccos(u)) \) are the Chebyshev polynomials and where the \( ' \) signifies that the first term of the sum must be halved. Moreover

\[
\left\| P_{2n+1}(x) - \frac{1}{x} \right\|_{[-b, -a] \cup [a, b]} \leq C \left( \frac{b - a}{b + a} \right)^n n \log n.
\]

(2.6)
Proof. We already noticed that 2.5 is being constructed through the process of Steps 1–4. Observe that in view of Corollary 2.1,

\[ E_n \left( \frac{1}{2((b^2-a^2)x + b^2 + a^2)}; [-1, 1] \right) \leq C \left( \frac{b-a}{b+a} \right)^n. \]  

(2.7)

Hence (2.6) follows from Theorem 2.2 and the construction (2.2) and (2.3). \( \square \)

Notice that (3.1) is essentially the rate of approximation of the polynomial (of degree \( 2n + 1 \)) of best approximation which is for all practical purposes impossible to find exactly.

Remark. Let \( b = 1 \) and \( a = \epsilon \). Then as \( \epsilon \to 0, \left( \frac{b-a}{b+a} \right) \to 1 \). That is to say the rate of approximation (2.6) decreases as the gap between the intervals tends to zero, which is intuitively plausible. It is also of interest to note that the above formula is appropriate to recover the coefficients of the polynomial, which is in general an ill-posed problem.

3 Discussion

Equation (2.5) is especially well suited for fast and accurate evaluation of \( P_{2n+1}(x) \).

We first remark that the integrand \( \frac{\cos(k\theta)}{2((b^2-a^2)\cos(\theta) + b^2 + a^2)} \) in (2.5) is smooth and periodic. Hence the Euler-McLaurin summation formula in conjunction with the trapezoidal rule allows accurate evaluation of the integral at low cost. See [13].

We can express \( P_{2n+1}(x) \) in the form \( P_{2n+1}(x) = \sum_{k=0}^{2n+1} a_k z^k \). We found, for computing purposes, that the Cauchy formula

\[ a_k = \frac{1}{2\pi i} \int_C \frac{P_{2n+1}(z)}{z^{k+1}} \; dz, \quad k = 0, 1, \ldots, 2n+1, \]

where the closed curve \( C \) encloses 0, was highly accurate and cost effective (again because of the smoothness and periodicity of the integrand).

Figure 3.1 shows how the 11-degree polynomial approximation over the intervals \([-2, -1] \cup [1, 2]\) compares to the actual function \( 1/x \). Note that the polynomial is defined outside of the intervals.

Equation (2.6), for small values of \( n \) (so that the factor \( \log n \) is neglected), and replacing \( P_{2n+1}(x) \) by \( P_n(x) \), takes the approximative form

\[ \left\| P_n(x) - \frac{1}{x} \right\| \leq C \left( \frac{b-a}{b+a} \right)^{n+1}. \]  

(3.1)

In the case \( a = 1, \ b = 2 \), the right hand side of (3.1) becomes \( C \frac{1}{3^{n+1}} \).
Figure 3.1: 11-degree polynomial approximation of $1/x$ over the intervals $x = [-2, -1] \cup [1, 2]$. The approximating polynomial $P_{11}(x)$ is represented by the continuous line.

From Table 3.1 we can infer that $E_k \approx C \frac{1}{3^{k-1}}$ with $C \approx 0.46$. This confirms the validity of the theoretical result (2.6) as well as of the accuracy of the implementation of equation (2.5).

We mention that we are aware of a technique that has been used by some authors consists of building a function $g(x)$ in such a way that the function $h(x)$ defined by

$$h(x) = \begin{cases} \frac{1}{x}, & x \in [-b, -a] \\ g(x), & x \in [-a, a] \\ \frac{1}{x}, & x \in [b, a] \end{cases}$$

is as smooth as possible and approximating the function $h(x)$ so obtained by poly-

| $k$ | $E_k = |P_k(x) - (\frac{1}{x})|$ |
|-----|-------------------------------|
| 3   | $2.9 \times 10^{-1}$          |
| 11  | $4 \times 10^{-3}$            |
| 19  | $1.2 \times 10^{-5}$          |
| 27  | $2.9 \times 10^{-7}$          |
nomials $P_n(x)$ on $[-b, b]$. Clearly if $P_n(x)$ approximates $h(x)$ on $[-b, b]$, then $P_n(x)$ approximates $\frac{1}{x}$ on $[-b, -a] \cup [a, b]$. However such an extension $h(x)$ is at best $C^\infty$ and cannot be analytic. It follows that the rate of approximation cannot decay exponentially fast. In fact it can be shown that no matter how smooth $h(x)$ is, the rate of approximation is at best $O\left(e^{-\sqrt{n}}\right)$ whereas (2.6) provides an exponential decay.

The technique described above for the approximation of $\frac{1}{x}$ can be modified to approximate any analytic function. We give below such an example of approximation of (different) constants on $[-b, -a] \cup [a, b]$. This problem occurs routinely in the design of digital filters. See [5] and [9].

**Theorem 3.1.** Let

$$h(x) = \begin{cases} 1, & x \in [a, b] \\ -1, & x \in [-b, -a]. \end{cases}$$

Then the polynomial of near best uniform approximation to $h(x)$ of degree $2n + 1$ on $[-b, -a] \cup [a, b]$ is given by

$$P_{2n+1}(x) = x \sum_{k=0}^{n} \frac{2}{\pi} \int_{0}^{\pi} \cos(k\theta) \frac{\cos(k\theta)}{\sqrt{\frac{1}{2}((b^2 - a^2)\cos(\theta) + b^2 + a^2)}} d\theta \times \left(T_k\left(\frac{2x^2}{b^2 - a^2} - \frac{b^2 + a^2}{b^2 - a^2}\right)\right).$$

4 Testing the Algorithm Numerically

In this section we present two kinds of numerical experiments. First, we analyse the case of a $4 \times 4$ matrix. We choose a small matrix because we expect the reader to easily check the results of the outcome of our calculations. The main thing we want to highlight is how well the polynomial approximation captures $A^{-1}$. We then try the algorithm on significantly larger matrices, with the aim of showing that the computation is numerically stable, and further, that the estimates on the error are accurate.

We choose the $4 \times 4$ symmetric matrix with eigenvalues $-1.8999721$, $-1.1000377$, $1.3000027$, $1.69999071$. We choose to approximate $1/x$ over the ranges $[-2, -1] \cup [1, 2]$, purposely choosing values that do not sharply enclose the eigenvalues. We compute $P_n(A)$ and compare it entry by entry to $A^{-1}$, and we denote by $E_n$ the maximum, in absolute value, of the errors for a polynomial of degree $n$. As evidenced by the error in Table 4.1 we see good agreement $s$ between $P_n(x)$ and $\frac{1}{x}$.

Comparing a matrix inverse and an approximation when the matrix is large and dense is not practical. Instead for the larger matrix tests we instead compute $\|AP(A)x - x\|_\infty$, for a few randomly chosen vectors $x$. These results are more stable and of course, also less costly, i.e. $O(m^2)$, where $m$ is the matrix size.
Table 4.1: Maximum error, entry by entry, between $P_n(A)$ and $A^{-1}$.

<table>
<thead>
<tr>
<th>Degree of $P_n(x)$</th>
<th>$E_n$</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>$4.266 \times 10^{-3}$</td>
</tr>
<tr>
<td>19</td>
<td>$2.002 \times 10^{-7}$</td>
</tr>
<tr>
<td>27</td>
<td>$3.033 \times 10^{-1}$</td>
</tr>
</tbody>
</table>

In the experiments we created matrices of different sizes with known eigenvalues. We keep the degree of the polynomial approximation fixed and increase the size $m$ of the matrix. The matrix is constructed by creating a diagonal matrix $D$ of random entries (eigenvalues), spanning 2 intervals over $x$. Using a QR algorithm one can then create independently an orthogonal matrix $Q$. The final symmetric positive definite matrix $A = Q^T D Q$ will have known eigenvalues.

We computed $\|A P(A) x - x\|_\infty$ using between five and seven different randomly chosen $m$-dimensional vectors $x$. We report below the averaged outcomes $\bar{A}_s$ for several values of the degree $s$ of the polynomial. For a 27 degree polynomial Table 4.2 shows how the results depend little on the size of the matrix. We see

Table 4.2: Averages on $x$ of the values $\|A P(A) x - x\|_\infty$. Polynomial of degree 27.

<table>
<thead>
<tr>
<th>$m$</th>
<th>$\bar{A}_{27}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000</td>
<td>$5.219 \times 10^{-7}$</td>
</tr>
<tr>
<td>5000</td>
<td>$5.602 \times 10^{-7}$</td>
</tr>
<tr>
<td>10000</td>
<td>$5.373 \times 10^{-7}$</td>
</tr>
</tbody>
</table>

that the error is about twice the error given on the last line of Table 3.1 for the approximation of $\frac{1}{x}$ by $P_{27}(x)$. Although we cannot explain this discrepancy we are satisfied because

1. The error is of the same order as that given on Table 3.1.
2. Table 4.2 shows that the error does not (significantly) increase with the size $n$ of the matrix, as predicted by the theory. (See (1.1).)

We now investigate how the results change if we use a different degree for the approximating polynomial. The experiment is the same, however, we try the cases of degree 19 and 11, respectively. We see in Tables 4.3 and 4.4, when compared to Table 4.2, excellent agreement.
Table 4.3: Averages on $x$ of the values $\|AP(A)x - x\|_\infty$. Polynomial of degree 19. Compare to Table 4.2.

<table>
<thead>
<tr>
<th>$m$</th>
<th>$\bar{A}_{19}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000</td>
<td>$3.266 \times 10^{-3}$</td>
</tr>
<tr>
<td>5000</td>
<td>$4.002 \times 10^{-3}$</td>
</tr>
<tr>
<td>10000</td>
<td>$4.033 \times 10^{-3}$</td>
</tr>
</tbody>
</table>

Table 4.4: Averages on $x$ of the values $\|AP(A)x - x\|_\infty$. Polynomial of degree 11. Compare to Table 4.2.

<table>
<thead>
<tr>
<th>$m$</th>
<th>$\bar{A}_{11}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000</td>
<td>$8.079 \times 10^{-3}$</td>
</tr>
<tr>
<td>5000</td>
<td>$7.692 \times 10^{-3}$</td>
</tr>
<tr>
<td>10000</td>
<td>$8.737 \times 10^{-3}$</td>
</tr>
</tbody>
</table>

5 Conclusions and Prospects

We summarize our work as follows. Given an invertible symmetric matrix $A$ whose eigenvalues are known to belong in the union of two intervals $[-b, -a] \cup [a, b]$, $0 < a < b$, we build a matrix preconditioner to $A$ of the form $P_n(A)$. Here $P_n(x)$ is the polynomial of degree $n$ of (near) best uniform approximation to $\frac{1}{x}$ on $[-b, -a] \cup [a, b]$.

The approximation of $P_n(x)$ to $\frac{1}{x}$ was shown to be very good and the cost involved in creating the polynomial is reasonable. Moreover we showed that the method can be cast as a practical and stable algorithm as demonstrated by the numerical experiments.

The problem of locating the extreme eigenvalues of $A$ with high accuracy is addressed in a separate paper (see [8]). However, we showed that it is not required to know any of the eigenvalues of $A$; it suffices to know the intervals described above where the eigenvalues are located.

The method works well if the following conditions are fulfilled:

1. We have estimates on location of the extreme eigenvalues.

2. The matrix should be “close to normal.”

Let us examine more closely the effect of non-normality which is closely related to the problem of simultaneous approximation of a function and its derivatives by a polynomial and its derivatives.

Approximation of $P_{27}^{(k)}(x)$ to $\left(\frac{1}{2}\right)^{(k)}$ on $[-2, -1] \cup [1, 2]$.

$\left|P_{27}^{(k)}(x) - \left(\frac{1}{2}\right)^{(k)}\right|$ signifies the sup norm on $[-2, -1] \cup [1, 2]$. 

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Table 5.1: Error between $P_{27}^{(k)}(x)$ and $(\frac{1}{x})^{(k)}$

<table>
<thead>
<tr>
<th>$k$</th>
<th>$P_{27}^{(k)}(x) - (\frac{1}{x})^{(k)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$2.9 \times 10^{-7}$</td>
</tr>
<tr>
<td>1</td>
<td>$5 \times 10^{-6}$</td>
</tr>
<tr>
<td>2</td>
<td>$6.2 \times 10^{-4}$</td>
</tr>
<tr>
<td>3</td>
<td>$9.1 \times 10^{-3}$</td>
</tr>
</tbody>
</table>

Let us examine now what may happens if $A$ is not normal.
Let the $n \times n$ matrix $A$ be as follows.

$$A = \begin{pmatrix}
    c & 1 & 0 & \ldots & 0 & 0 \\
    0 & c & 1 & \ldots & 0 & 0 \\
    0 & 0 & c & 1 & \ldots & 0 \\
    \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
    0 & 0 & \ldots & 0 & 0 & c
\end{pmatrix}$$

This matrix is “very far” from normal.

Let $f(z)$ be analytic on a domain containing $c$. Then

$$f(A) = \begin{pmatrix}
    f(c) & f'(c) & \ldots & \ldots & \frac{f^{(n-1)}(c)}{(n-1)!} \\
    0 & f(c) & f'(c) & \ldots & \ldots \\
    0 & 0 & f(c) & f'(c) & \ldots & \ldots \\
    \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
    0 & 0 & \ldots & 0 & 0 & f(c)
\end{pmatrix}$$

Let now $P(z)$ approximate $f(z)$ on a domain containing the eigenvalue $c$. Then the approximation of $f(A)$ by $P(A)$ will be

$$P(A) = \begin{pmatrix}
    P(c) & P'(c) & \ldots & \ldots & \frac{P^{(n-1)}(c)}{(n-1)!} \\
    0 & P(c) & P'(c) & \ldots & \ldots \\
    0 & 0 & P(c) & P'(c) & \ldots & \ldots \\
    \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
    0 & 0 & \ldots & 0 & 0 & P(c)
\end{pmatrix}$$

It is now clear that if the approximation $|P^{(k)}(x) - f^{(k)}(x)|$ is poor so will be the approximation of $f(A)$ by $P(A)$.

We presented above the first stage of a project. The next step will consist of obtaining estimates on the size and location of the intervals containing the eigenvalues of $A$. This is investigated in [8]. If the eigenvalues are located in $[a, b] \cup [c, d]$, $b - a \neq d - c$, we can always use the method described above by enlarging, if necessary, the smallest of the two intervals so as its length equals the length of the other interval.

However, especially in the case where there is a significant discrepancy between the lengths of the intervals, it is of interest to leave the intervals unchanged and to find the (near) best approximation to $\frac{1}{2}$ on $[a, b] \cup [c, d]$. We plan to investigate the possible use of the Fekete (or Leja) points to achieve this purpose. We refer the reader to [10].

The technique consists first to find the equilibrium location of $n$ “electrons” on $[a, b] \cup [c, d]$, where $n$ is the degree of the polynomial. This is, theoretically, achieved through the following procedure.
Let \( \Gamma = [a, b] \cup [c, d] \), \( n \in \mathbb{N}, \ z_0, z_1, \ldots, z_n \in \Gamma \).

Find \( z_i \in \Gamma \) in such a way that

\[
\prod_{0 \leq i < j \leq n} |z_i - z_j|
\]

is maximized. (Hence the “electrons” are “2 - D electrons.”) We display in Figure 5.1 the graphical solution of this problem in the case of 60 electrons located in \([-2, -0.2] \cup [0.2, 2]\). Because the electrons repel each other we witness, as expected, a clustering of the electrons near the end points -2 and 2. What was maybe not as easy to predict is a slight reclustering of the electrons near the inner points -0.2 and 0.2.

However our efforts to find the location of the points \( z_i \) in the general case of intervals of different lengths have been unsuccessful. The first step in this process consists of finding for a given aspect ratio \( \frac{b-a}{c-d} \) the proportion of electrons located in one (and so in both) of the intervals. The answer to this question is not known.

Once this is established the location of the electrons is determined by (5.1) Once the points \( z_i \) are found the approximation polynomial will be obtained by interpolation, using the familiar formula for the polynomial \( P_n(z) \) interpolating \( f(z) \) at the points \( z_k \).

\[
P_n(z) = \sum_{k=0}^{n} f(z_k) \prod_{i=0, i \neq k}^{n} \left( \frac{z - z_i}{z_k - z_i} \right),
\]

with \( f(z) = \frac{1}{z} \).

Another possible approach to building the optimal polynomial in the case of intervals of different lengths consists of building an appropriate Green’s function with logarithmic pole at infinity. To be more precise the polynomials (2.5) were built in Section 2 with Fourier series techniques. However these techniques are successful precisely in the setting where the intervals are of equal lengths.
However the “trick” of approximating $\frac{1}{x}$ on $[a^2, b^2]$ hides in fact something deeper. Indeed it can be shown that

$$G(z) = \frac{1}{2} \log \left| \frac{2z^2}{b^2 - a^2} - \frac{b^2 + a^2}{b^2 - a^2} + \sqrt{\left( \frac{2z^2}{b^2 - a^2} - \frac{b^2 + a^2}{b^2 - a^2} \right)^2 - 1} \right|$$

is the solution of the steady-state $2-D$ heat equation with temperature being held at zero on the two intervals and with a unit impulse of heat at $\infty$. The polynomials (2.5) could have been also obtained with the aid of this Green’s function. Now, however, we can modify this Green’s function in such a way that it corresponds to the solution of the steady-state $2-D$ heat equation on intervals of different lengths. We are now in the process of investigating the extend to which this modified Green’s function can be used to adapt (2.5) in the case of intervals of different lengths.
Acknowledgments

The authors wish to express their appreciation to James Hyman and Rob Indik for very fruitful discussions. JMR is supported by a DOE “Early Career” grant DE-FG02-02ER25533. JMR also thanks T7 at Los Alamos, where much of this work was performed. MH was supported by a NSF/VIGRE fellowship.

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