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Chebyshev Semi-Discrete Approximations for Linear Parabolic Problems*)**)

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1. Introduction

Consider the solution $u(x, t)$ of the heat equation

$$(1.1)\qquad \begin{cases} u_t(x,t) = u_{xx}(x,t) + r(x), & 0<x<1,\ t>0, \\ u(x,0) = \tilde{u}(x), & 0\leqq x\leqq 1, \\ u(0,t) = u(1,t) = 0, & t>0. \end{cases}$$

Leaving time continuous, consider the particular spatial discretization of (1. 1) brought about by the usual three-point difference approximation to u_{xx}, i.e.,

$$u_{xx}(ih, t) \doteq \frac{u((i+1)h, t) - 2u(ih, t) + u((i-1)h, t)}{h^2} \qquad ((N+1)h = 1).$$

The resulting approximation $w(ih, t)$ to the solution $u(x, t)$ of (1. 1), called the *semi-discrete* approximation of $u(x, t)$, satisfies

$$(1.2)\qquad \begin{cases} \dfrac{dw(ih,t)}{dt} = \dfrac{w((i+1)h,t) - 2w(ih,t) + w((i-1)h,t)}{h^2} + r(ih), & 1\leqq i\leqq N,\ t>0, \\ w(ih,0) = \tilde{u}(ih), & 0\leqq i\leqq N+1, \\ w(0,t) = w((N+1)h,t) = 0, & t>0. \end{cases}$$

Written equivalently in matrix notation, this becomes

$$(1.3)\qquad \begin{cases} \dfrac{d\mathbf{w}(t)}{dt} = -A\mathbf{w}(t) + \mathbf{r}, & t>0, \\ \mathbf{w}(0) = \tilde{\mathbf{u}}, \end{cases}$$

where $\mathbf{w}(t)$, $\mathbf{r}$, and $\tilde{\mathbf{u}}$ are column vectors with N components, with $\mathbf{w}(t) = (w_1(t), \ldots, w_N(t))^T$ where $w_i(t) \equiv w(ih, t)$. Note that $\mathbf{r}$ and $\tilde{\mathbf{u}}$ are determined from

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**) The contents of this paper also can be found in [12, Ch. 9].

given quantities, and A is the familar tridiagonal Hermitian and positive definite $N \times N$ matrix, given by

$$A = \frac{1}{h^2}\begin{bmatrix} 2 & -1 & & & 0 \\ -1 & 2 & -1 & & \\ & \cdot & \cdot & \cdot & \\ & & \cdot & \cdot & \cdot \\ & & & \cdot & \cdot \;\; -1 \\ 0 & & & -1 & 2 \end{bmatrix} \tag{1.4}$$

In what is to follow, only the Hermitian positive definite character of the $N \times N$ matrix A is essential, *and we henceforth assume that our semi-discretization results in* (1. 3) *with A Hermitian and positive definite.* In particular, this assumption is valid for linear parabolic problems in n spatial variables of the form

$$\begin{cases} u_t(x, t) = \sum_{i=1}^{n} (K_i(x) u_{x_i}(x, t))_{x_i} - \sigma(x) u(x, t) + r(x), & \text{for } \; t > 0, \; x \in \Omega, \\ u(x, 0) = \tilde{u}(x), & x \in \Omega, \\ u(x, t) = g(x), & x \in \partial\Omega, \; t > 0, \end{cases} \tag{1.5}$$

where Ω is a bounded region in R^n, and the quantities $K_i(x)$, $\sigma(x)$, are positive in $\bar{\Omega}$, provided that a suitable $(2n+1)$-point difference approximation of (1. 5) is used (cf. [10, p. 253]).

Returning to (1. 3), the solution $\mathbf{w}(t)$ can obviously be expressed as

$$\mathbf{w}(t) = A^{-1}\mathbf{r} + \exp(-tA)\{\tilde{\mathbf{u}} - A^{-1}\mathbf{r}\} \qquad (t \geqq 0), \tag{1.6}$$

where as usual, $\exp(-tA) \equiv \sum_{k=0}^{\infty} (-tA)^k/k!$. The solution of (1. 6) is commonly approximated by means of matrix Padé rational approximations of $\exp(-tA)$, and these give, as special cases, the well-known forward difference, backward difference, and Crank—Nicolson methods for such parabolic problems (cf. [10, § 8. 3]). Our interest in the next section will be on *Chebyshev*, rather than *Padé*, rational approximations of $\exp(-tA)$. This is because Padé rational approximations of e^{-x}, being defined as *local* approximations of e^{-x} at $x=0$, are generally poor approximations of e^{-x} for large x, and this leads to restrictions (for reasons of stability and/or accuracy) on the time step that can be taken. Chebyshev rational approximations of e^{-x}, in contrast, are defined *globally* with respect to the interval $[0, +\infty)$, and do not have such time step restrictions, as we shall see.

2. Chebyshev semi-discrete approximations

To define the Chebyshev semi-discrete approximations of (1. 6), we consider the following approximation problem. If π_m denotes all real polynomials $p(x)$ of degree at most m, and $\pi_{m,n}$ analogously denotes all real rational functions $r_{m,n}(x)=$ $=p(x)/q(x)$ with $p\in\pi_m$, $q\in\pi_n$, then let

(2. 1) $$\lambda_{m,n}\equiv\inf_{\pi_{m,n}}\|e^{-x}-r_{m,n}(x)\|_{L_\infty[0,\infty]}=\inf_{\pi_{m,n}}\{\sup_{x\geqq 0}|e^{-x}-r_{m,n}(x)|\}.$$

These constants $\lambda_{m,n}$ are called the *Chebyshev constants for* e^{-x} with respect to the interval $[0, +\infty)$. It is obvious that $\lambda_{m,n}$ is finite if and only if $0\leqq m\leqq n$, and moreover, given any pair (m, n) of nonnegative integers with $0\leqq m\leqq n$, it is known (cf. ACHIESER [1, p. 55]) that, after dividing out possible common factors, there exists a unique $\hat{r}_{m,n}\in\pi_{m,n}$ with

(2. 2) $$\hat{r}_{m,n}(x)=\hat{p}_{m,n}(x)/\hat{q}_{m,n}(x)$$

and with $\hat{q}_{m,n}(x)>0$ on $[0, \infty)$, such that

(2. 3) $$\lambda_{m,n}=\|e^{-x}-\hat{r}_{m,n}(x)\|_{L_\infty[0,\infty]}.$$

Since $\hat{q}_{m,n}(tA)=\sum_{j=0}^{n}c_j(tA)^j$ is a real polynomial in the $N\times N$ matrix A, it is evident from the fact that $\hat{q}_{m,n}(x)$ is positive on $[0, +\infty)$ that $\hat{q}_{m,n}(tA)$ is a Hermitian and positive definite $N\times N$ matrix for each $t\geqq 0$. Thus, in analogy with (1. 6), we define the *(m, n)-th Chebyshev semi-discrete approximation* $\mathbf{w}_{m,n}(t)$ of the solution $\mathbf{w}(t)$ of (1. 3) as

(2. 4) $$\mathbf{w}_{m,n}(t)=A^{-1}\mathbf{r}+(\hat{q}_{m,n}(tA))^{-1}(\hat{p}_{m,n}(tA))\{\tilde{\mathbf{u}}-A^{-1}\mathbf{r}\}\qquad(t\geqq 0).$$

For the practical computation of $\mathbf{w}_{m,n}(t)$ for a fixed finite $t\geqq 0$, assume first that the steady-state solution $\hat{\mathbf{w}}\equiv A^{-1}\mathbf{r}$ of (1. 3) has been determined, which amounts to solving the matrix equation $A\hat{\mathbf{w}}=\mathbf{r}$. Then, we write (2. 4) equivalently as

(2. 5) $$\hat{q}_{m,n}(tA)\mathbf{w}_{m,n}(t)=\mathbf{v}_0;\quad \mathbf{v}_0\equiv\hat{q}_{m,n}(tA)\hat{\mathbf{w}}+\hat{p}_{m,n}(tA)\{\tilde{\mathbf{u}}-\hat{\mathbf{w}}\},$$

where $\mathbf{v}_0$ is determined from the known initial vector $\tilde{\mathbf{u}}$ (cf. (1. 3)), and the known steady-state vector $\hat{\mathbf{w}}=A^{-1}\mathbf{r}$. Since $\hat{q}_{m,n}\in\pi_n$ is positive on $[0, +\infty)$, $\hat{q}_{m,n}$ can be factored into real linear and quadratic factors:

(2. 6) $$\hat{q}_{m,n}(x)=\prod_{i=1}^{s_1}l_i(x)\cdot\prod_{j=1}^{s_2}m_j(x),\quad s_1+2s_2=n,$$

where $l_i\in\pi_1$, $m_j\in\pi_2$, and where the l_i and m_j are also positive on $[0, +\infty)$. Thus, the matrices $l_i(tA)$ and $m_j(tA)$ are again Hermitian and positive definite for each

$t \geqq 0$, and the solution $\mathbf{w}_{m,n}(t)$ of (2. 5) can be obtained by solving recursively the matrix problems

$$\text{(2. 7)} \qquad \begin{cases} m_j(tA)\mathbf{v}_j = \mathbf{v}_{j-1}, & 1 \leqq j \leqq s_2, \\ l_i(tA)\mathbf{v}_{s_2+i} = \mathbf{v}_{s_2+i-1}, & 1 \leqq i \leqq s_1, \end{cases}$$

and then defining $\mathbf{w}_{m,n}(t) \equiv \mathbf{v}_{s_2+s_1}$. In particular, when A is tridiagonal as in (1. 4), the matrices of (2. 7) are either tridiagonal or five-diagonal positive definite matrices. As such, the solution of (2. 7) by means of Gaussian elimination with no pivoting is both computationally fast and numerically accurate.

For computational efficiency, one should always choose $m=n$ in (2. 4) for applications of the Chebyshev semi-discrete method to actual problems. The reason for this is quite clear: the bulk of the work in finding the solution $\mathbf{w}_{m,n}(t)$ of (2. 5) comes from the inversion of the polynomial $\hat{q}_{m,n}(tA)$ of degree n in the matrix A, and the work involved in this inversion in practice is virtually independent of the choice of m. For further discussion of such computational aspects of the Chebyshev semi-discrete method, see [11].

To estimate the error in $\mathbf{w}(t)-\mathbf{w}_{m,n}(t)$ we use vector l_2-norms, i.e., if $\mathbf{v} = (v_1, \ldots, v_N)^T$, then $\|\mathbf{v}\|_2^2 \equiv \sum_{i=1}^{N} |v_i|^2$. If, for any $N \times N$ matrix C, $\|C\|_2$ denotes the induced operator norm (or spectral norm) of C, i.e.,

$$\text{(2. 8)} \qquad \|C\|_2 \equiv \sup_{\mathbf{v} \neq \mathbf{0}} \left\{ \frac{\|C\mathbf{v}\|_2}{\|\mathbf{v}\|_2} \right\},$$

it is well known (cf. [10, p. 11]) when C is Hermitian with (real) eigenvalues μ_i, $1 \leqq i \leqq N$, that $\|C\|_2$ can be expressed as

$$\text{(2. 9)} \qquad \|C\|_2 = \max_{1 \leqq i \leqq N} |\mu_i|.$$

Consequently, if $\{\lambda_i\}_{i=1}^N$ denotes the (positive) eigenvalues of A, the assumed Hermitian character of A allows us to conclude from (2. 9) that

$$\text{(2. 10)} \qquad \|\exp(-tA) - \hat{r}_{m,n}(tA)\|_2 = \max_{1 \leqq i \leqq N} |e^{-t\lambda_i} - \hat{r}_{m,n}(t\lambda_i)|, \quad \text{for all} \quad t \geqq 0.$$

But as $t\lambda_i \geqq 0$ for all $1 \leqq i \leqq N$ and for all $t \geqq 0$, it follows from (2. 3) that

$$\|\exp(-tA) - \hat{r}_{m,n}(tA)\|_2 \leqq \lambda_{m,n}, \quad \text{for all} \quad t \geqq 0.$$

Consequently, from (1. 6) and (2. 4),

$$\text{(2. 11)} \qquad \|\mathbf{w}(t) - \mathbf{w}_{m,n}(t)\|_2 \leqq \|\exp(-tA) - \hat{r}_{m,n}(tA)\|_2 \cdot \|\tilde{\mathbf{u}} - A^{-1}r\|_2 \leqq \leqq \lambda_{m,n} \|\tilde{\mathbf{u}} - A^{-1}r\|_2, \quad \text{for all} \quad t \geqq 0.$$

Note that since the right-hand side of (2. 11) is *independent* of t, we have an error bound for $\mathbf{w}(t)-\mathbf{w}_{m,n}(t)$ for *all* $t \geqq 0$. In contrast with the familiar Padé methods which restrict the size of t for reasons of accuracy and/or stability, the Chebyshev semi-discrete method can be used for very large values of t. The difference, of course, comes from the fact that Padé rational approximations of e^{-x} are designed to approximate e^{-x} well in a neighbourhood of $x=0$, whereas Chebyshev rational approximations of e^{-x} are designed to approximate e^{-x} over $[0, +\infty)$.

In general, the error of the spatial discretization leading to (1. 3) must be bounded to give the total error (i.e., space and time) of these Chebyshev semi-discrete approximations. Such spatial discretization errors are discussed in [12], for example.

3. The Chebyshev constants for e^{-x}

The utility of the Chebyshev semi-discrete approximations depends, from (2. 11), on the behavior of the Chebyshev constants $\lambda_{m,n}$ of (2. 1), as $n \to \infty$. From (2. 1), it is clear that

$$0 < \lambda_{n,n} \leqq \lambda_{n-1,n} \leqq \cdots \leqq \lambda_{0,n} \qquad (n \geqq 0). \tag{3. 1}$$

Based on elementary arguments, the following result was proved in Cody, Meinardus, and Varga [4].

Theorem 1. *Let $\{m(n)\}_{n=0}^{\infty}$ be any sequence of nonnegative integers with $0 \leqq m(n) \leqq n$ for each $n \geqq 0$. Then,*

$$\overline{\lim_{n \to \infty}} \, (\lambda_{m(n),n})^{1/n} \leqq \frac{e^{-\alpha}}{2} < \frac{1}{2}, \tag{3. 2}$$

where $\alpha = 0.13923\ldots$ is the real solution of $2\alpha e^{2\alpha+1} = 1$. Moreover,

$$\underline{\lim_{n \to \infty}} \, (\lambda_{0,n})^{1/n} \geqq \frac{1}{6}. \tag{3. 3}$$

The results of (3. 2) and (3. 3) establish the *geometric convergence to zero* of the Chebyshev constants $\lambda_{m,n}$ for e^{-x} in $[0, \infty)$. In particular, if $m(n)=n$, then the Chebyshev constants $\lambda_{n,n}$ for e^{-x} in $[0, +\infty)$ are from [4]:

n	$\lambda_{n,n}$
0	5.00(−01)
1	6.69(−02)
2	7.36(−03)
3	7.99(−04)
4	8.65(−05)

n	$\lambda_{n,n}$
5	9.35(−06)
6	1.01(−06)
7	1.09(−07)
8	1.17(−08)
9	1.26(−09)

n	$\lambda_{n,n}$
10	1.36(−10)
11	1.47(−11)
12	1.58(−12)
13	1.70(−13)
14	1.83(−14)

,

where $\alpha(-\beta)$ denotes $\alpha \cdot 10^{-\beta}$ in the table above. Thus, the rate of convergence to zero of the $\lambda_{n,n}$ appears to be much better than that given by the upper bound of (3. 2). Also, the quantities $\lambda_{0,n}$, $0 \leqq n \leqq 9$, as tabulated in [4], would lead one to conjecture that $\lim_{n\to\infty} (\lambda_{0,n})^{1/n}$ exists, and that

$$\lim_{n\to\infty} (\lambda_{0,n})^{1/n} = \frac{1}{3}. \tag{3.4}$$

This in fact has been recently shown by SCHÖNHAGE [8].

4. Chebyshev constants for other entire functions

The preceeding results on the geometric convergence to zero of the Chebyshev constants $\lambda_{m,n}$ for $1/e^x$ in (3. 2) and (3. 3) hold for a wider class of entire functions than just $f(z)=e^z$. A generalization of the results of Theorem 1 has been recently given in MEINARDUS and VARGA [7], and can be described as follows.

Let $f(z) = \sum_{k=0}^{\infty} a_k z^k$ be an entire function (i.e., analytic for every finite z) with $M_f(r) \equiv \sup_{|z|=r} |f(z)|$ its maximum modulus function. Then, f is of *perfectly regular growth* (ϱ, β) (cf. BOAS [2, p. 8] and VALIRON [9, p. 45]) if there exist two (finite) positive numbers ϱ (the order) and B (the type) such that

$$\lim_{r\to\infty} \frac{\ln M_f(r)}{r^\varrho} = B. \tag{4.1}$$

We then have (cf. [7])

THEOREM 2. *Let* $f(z) = \sum_{k=0}^{\infty} a_k z^k$ *be an entire function of perfectly regular growth* (ϱ, B) *with* $a_k \geqq 0$ *for all* $k \geqq 0$, *and for any pair* (m, n) *of nonnegative integers with* $0 \leqq m \leqq n$, *let*

$$\lambda_{m,n} \equiv \inf_{\pi_{m,n}} \left\| \frac{1}{f(x)} - r_{m,n}(x) \right\|_{L_\infty[0,\infty]} \tag{4.2}$$

be its associated Chebyshev constants. Then, for any sequence $\{m(n)\}_{n=0}^{\infty}$ *of nonnegative integers with* $0 \leqq m(n) \leqq n$ *for each* $n \geqq 0$,

$$\overline{\lim_{n\to\infty}} (\lambda_{m(n),n})^{1/n} \leqq 2^{-1/\varrho} < 1. \tag{4.3}$$

Moreover,

$$\underline{\lim_{n\to\infty}} (\lambda_{0,n})^{1/n} \geqq 2^{-2-1/\varrho}. \tag{4.4}$$

As special cases of Theorem 2, we have of course $f(z)=e^z$, $f(z)=\sinh(z^p)$ and $f(z)=J_p(iz)$ for p a nonnegative integer, where J_p denotes the Bessel function of the first kind. For $f(z)=e^z$, for which $\varrho=B=1$ in (4. 1), the results of (4. 3) and (4. 4) are slightly weaker than those of (3. 2) and (3. 3) of Theorem 1.

The proofs of Theorems 1 and 2 depend upon estimating

$$\frac{1}{s_n(x)}-\frac{1}{f(x)}$$

where $s_n(z)=\sum_{k=0}^{n} a_k z^k$ is the n-th partial sum of $f(z)$. It is shown in [7] that, under the hypotheses of Theorem 2,

$$\lim_{n\to\infty}\left(\left\|\frac{1}{s_n}-\frac{1}{f}\right\|_{L_\infty[0,\infty]}\right)^{1/n}=2^{-1/\varrho},$$

so that the upper bound of (4. 3) cannot be improved using this specific technique.

Upon examining Theorem 2, we see that the bounds of (4. 3) and (4. 4) depend upon ϱ, but not on B, and this suggests the possibility of extensions of Theorem 2 to entire functions which are of finite order, but not of perfectly regular growth. Such extensions have been considered in MEINARDUS, REDDY, TAYLOR, and VARGA [6], and we state a representative result which generalizes Theorem 2. For notation, let $\varepsilon(r,s)$, for given $r>0$ and $s>1$, denote the unique open ellipse in the complex plane with foci at $x=0$ and $x=r$ and semi-major and semi-minor axes a and b such that $b/a=(s^2-1)/(s^2+1)$. If $f(z)$ is any entire function, we set

$$\tilde{M}_f(r,s)=\sup\{|f(z)|: z\in\varepsilon(r,s)\}. \tag{4. 5}$$

THEOREM 3. *Let $f(z)=\sum_{k=0}^{\infty} a_k z^k$ be an entire function with nonnegative Taylor coefficients and $a_0>0$. If there exist real numbers $s>1$, $A>0$, $\theta>0$ and $r_0>0$ such that*

$$\tilde{M}_f(r,s)\leqq A(\|f\|_{L_\infty[0,r]})^{\theta}\quad\text{for all}\quad r\geqq r_0, \tag{4. 6}$$

then there exist a real number $q\geqq s^{1/(1+\theta)}>1$ and a sequence of real polynomials $\{p_n(x)\}_{n=0}^{\infty}$ with $p_n\in\pi_n$ for each $n\geqq 0$ such that

$$\overline{\lim_{n\to\infty}}\left\{\left\|\frac{1}{f(x)}-\frac{1}{p_n(x)}\right\|_{L_\infty[0,\infty]}\right\}^{1/n}=\frac{1}{q}<1. \tag{4. 7}$$

Note that (4. 7) implies the geometric convergence to zero of the Chebyshev constants $\{\lambda_{m(n),n}\}_{n=0}^{\infty}$ of $1/f$ when $0\leqq m(n)\leqq n$.

To motivate the next result, it is convenient to recall some classical results of Bernstein for polynomial approximation on *finite* intervals. Given a real-valued function $f\in C^0[-1,+1]$, let

$$E_n(f)\equiv\inf_{\pi_n}\|f-p_n\|_{L_\infty[-1,+1]}. \tag{4. 8}$$

If f is the restriction to $[-1,+1]$ of a function analytic in an ellipse in the complex plane with foci -1 and $+1$, then Bernstein proved (cf. MEINARDUS [5, p. 91]) that there exists a real number $q>1$ such that

$$\overline{\lim_{n\to\infty}}\, E_n^{1/n}(f) = \frac{1}{q} < 1. \tag{4.9}$$

Conversely, if (4.9) holds, Bernstein proved the *inverse* result (cf. MEINARDUS [5, p. 92]) that f is necessarily the restriction to $[-1, +1]$ of a function analytic in an ellipse in the complex plane with foci at -1 and $+1$. Consider then the results of of Theorems 2 and 3. These give *sufficient* conditions on the entire function $f(z)$ so that the Chebyshev constants $\lambda_{m,n}$ of $1/f$, for $0\leqq m\leqq n$, converge geometrically to zero as $n\to\infty$. In the spirit of Bernstein's classical inverse theorems, the following result of [6] gives *necessary* conditions for this geometric convergence.

THEOREM 4. *Let $f(x)>0$ be a real continuous function on $[0, \infty)$, such that there exist a sequence of real polynomials $\{p_n(x)\}_{n=0}^{\infty}$ with $p_n\in\pi_n$ for all $n\geqq 0$, and a real number $q>1$ such that*

$$\overline{\lim_{n\to\infty}} \left(\left\| \frac{1}{p_n} - \frac{1}{f} \right\|_{L_\infty[0,\infty]} \right)^{1/n} = \frac{1}{q} < 1. \tag{4.10}$$

Then, there exists an entire function $F(z)$ with $F(x)=f(x)$ for all $x\geqq 0$. Moreover, F is of finite order, i.e.,

$$\overline{\lim_{r\to\infty}} \frac{\ln\ln M_F(r)}{\ln r} = \varrho < \infty.$$

In addition, for each $s>1$, there exist real numbers $K=K(q, s)>0$, $\theta=\theta(q, s)>1$, and $r_0=r_0(q, s)>0$ such that

$$\tilde{M}_F(r, s) \leqq K(\|f\|_{L_\infty[0,r]})^{\theta} \quad \textit{for all} \quad r\geqq r_0. \tag{4.11}$$

Finally, to complement the preceding results of this section, it is shown in [6] that there exist entire functions $f(z)$, of finite order which are positive on $[0, +\infty)$, for which the Chebyshev constants $\lambda_{m,n}$ of $1/f$, for $0\leqq m\leqq n$, *cannot* converge geometrically to zero as $n\to\infty$.

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