On the maximum-norm of the restricted denominator approximations

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Abstract

In this paper we analyze the restricted denominator approximation method, which is a one parameter family of functions approximating the exponential function. We give a necessary and sufficient condition for the A-stability of the functions. We provide an estimate for the stability constant in the maximum-norm when the method applied to the one-dimensional heat-equation both on finite and on infinite interval.

1 Introduction

The so called restricted denominator approximations (RDA), a one parameter family of rational functions [1], are of the form

$$r_\theta(z) := \frac{1 + (1-2\theta)z}{(1-\theta z)^2}, \ \theta \in \mathbb{R}.$$

We say that a rational function r *approximates the exponential function of order* $p \geq 1$ if

$$r(z) = \exp(z) + O(z^{p+1}), \text{ as } z \to 0.$$

[1]This method is different from the well known θ-method with functions $r_\theta(z) = \frac{1+(1-\theta)z}{1-\theta z}$.

For $\theta = 1+\frac{1}{2}\sqrt{2}$ and $\theta = 1-\frac{1}{2}\sqrt{2}$ the function r_θ approximates the exponential function of order $p = 2$, for all other values of θ the order is $p = 1$ (see e.g. [6] and [9]). The RDA method can be used for the time discretization of initial value problems.

The solution of the one-dimensional heat equation on the whole real line

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2},\ x \in \mathbb{R},\ t \geq 0, \quad u(x,0) = u_0(x),\ x \in \mathbb{R},$$

via the RDA method leads to the one step iterative method

$$U^n = r_\theta(\tau A)U^{n-1},\ n = 1, 2, ..., \tag{1}$$

where τ is the time discretization step-size. Here

$$A := \frac{1}{h^2}\text{tridiag}[1, -2, 1],$$

where h is the space discretization step-size. The approximations are sequences $U^n = \{U_j^n\}_{j=-\infty}^{+\infty} \sim \{u(jh, n\tau)\}_{j=-\infty}^{+\infty}$ of numbers and U^0 is defined from $u_0(x)$.

Recall that a rational function r is called A-stable if

$$|r(z)| \leq 1,\ \text{for}\ \frac{\pi}{2} \leq \arg(z) \leq \frac{3\pi}{2}.$$

Later in this paper we show that for $\theta \in [1 - \frac{1}{2}\sqrt{2}, 1 + \frac{1}{2}\sqrt{2}]$ the corresponding functions r_θ are A-stable. Let l_∞ be the Banach space of infinite complex sequences $z = \{z_j\}_{j=-\infty}^{+\infty}$ endowed with the maximum norm $||z||_\infty = \sup_{\infty<j<+\infty} |z_j|$. In [7] it is shown that for all $\arg(z) < \pi$ the resolvent $R(z, A) = (zI - A)^{-1}$ exists and the inequality

$$||R(z, A)||_\infty \leq \frac{1}{|z| \cos \frac{\arg(z)}{2}}. \tag{2}$$

holds[2]. Hence $A : l_\infty \to l_\infty$ is a sectorial operator. Therefore, since the functions r_θ are A-stable for $\theta \in [1 - \frac{1}{2}\sqrt{2}, 1 + \frac{1}{2}\sqrt{2}]$, the numerical methods $r_\theta(\tau A)$ are stable (see e.g. [10]), i.e., $\sup_{n,\tau\geq 0} ||r_\theta^n(\tau A)||_\infty <$

[2]In fact, in [7] the inequality (2) was shown for the matrix tridiag$[1, -2, 1]$, but then it is also true for the matrix $A = \frac{1}{h^2}\text{tridiag}[1, -2, 1]$).

∞. Since the resolvent estimate in (2) is uniform in h the number $C_\theta := \sup_{n,\tau,h\geq 0} ||r_\theta^n(\tau A)||_\infty < \infty$. We will call the constant C_θ the *stability constant* of $r_\theta(\tau A)$. Note that by the argument in [4], this stability constant C_θ is an upper bound for the stability constant for the heat equation on a finite interval along with the Dirichlet or Neumann boundary conditions. In this paper we will give both an upper and a lower bound for C_θ.

We say that a numerical scheme $r(\tau A)$ is *unconditionally contractive in the maximum norm* if for all $\tau > 0$

$$||r(\tau A)||_\infty \leq 1, \tag{3}$$

or, equivalently, the corresponding sequence $U^n = r(\tau A)U^{n-1}$ satisfies

$$||U^n||_\infty \leq \max_{0\leq j\leq n-1}\{||U^j||_\infty\}, \text{ for } n \geq 0. \tag{4}$$

If (3) holds for only $\tau \in (0, \hat{\tau}]$ then we say that the the scheme is *conditionally conractive in the maximum norm.* We note, that the contractivity in the maximum norm is a natural requirement since the solution of the heat equation also satisfies the continuous form of (4). In [9] it is shown that if r is of order $p > 1$ then the scheme $r(\tau A)$ cannot be unconditionally contractive in the maximum norm. It is shown in [6] that the RDA method can be contractive in the maximum norm only for $\theta \in [0, 1]$, moreover, $||r_\theta(\tau A)||_\infty \leq 1$ for

$$\tau \in [0, h^2(2-6\theta)^{-1}], \quad \text{if } \theta \in [0, \tfrac{1}{3}) \tag{5}$$

$$\tau \in [0, \infty), \quad \text{if } \theta \in [\tfrac{1}{3}, 1] \tag{6}$$

The RDA method has both advantages and disadvantages. Since $r_\theta(\infty) = 0$, there are error estimates also for nonsmooth initial data, contrary to the famous second order Crank-Nicolson (CN) scheme (see e.g. [10]). If we consider the also second order scheme $r_{1-\frac{1}{2}\sqrt{2}}(\tau A)$ then from (6) we see that it is contractive in the maximum norm if $\tau \leq 4.12h^2$ while the CN method is contractive in the maximum norm only if $\tau \leq 1.5h^2$ (see e.g. [6]). Also, as we will show in Section 4, if we consider the heat equation on a bounded interval the RDA method is also contractive for τ large enough, which is again not true for the CN method. On the other hand the use of the RDA method requires the solution of two linear systems at each time step which is a big computational disadvantage.

The paper is organized as follows. In Section 2, we show that the functions r_θ are A-stable if and only if the parameter θ lies in the interval $[1-\frac{1}{2}\sqrt{2}, 1+\frac{1}{2}\sqrt{2}]$. In Section 3, we give a lower bound, in Section 4 we provide an upper bound for the stability constant in the maximum-norm of the RDA method when it is applied to the one-dimensional heat-equation on the whole real line. Also in Section 4, we give an estimate for $||r_\theta(\tau A)^n||_\infty$ when the RDA method is applied to the one-dimensional heat-equation on a finite interval. We show that in this case $||r_\theta(\tau A)^n||_\infty < 1$ if τ is large enough for all $\theta \in \mathbb{R}$.

2 A-stability of the restricted denominator approximations

In this section we derive a necessary and sufficient condition for the values of θ for the A-stability of the RDA method.

Theorem 2.1 *The function r_θ is A-stable if and only if*

$$\theta \in [1 - \frac{1}{2}\sqrt{2}, 1 + \frac{1}{2}\sqrt{2}]. \tag{7}$$

Proof. First, we show the sufficiency. Let $z = |z|e^{i\psi}$. Then for all complex number z and for all $\psi \in [\frac{\pi}{2}, \frac{3\pi}{2}]$ the following inequality has to be satisfied:

$$|r_\theta(z)|^2 = \frac{1 + (1-2\theta)^2|z|^2 + 2(1-2\theta)|z|\cos\psi}{(1+\theta^2|z|^2 - 2\theta|z|\cos\psi)^2} \leq 1,$$

which yields the condition

$$1 - |z|\frac{\theta^4|z|^3 - 4\theta^3\cos\psi|z|^2 + (4\theta^2\cos^2\psi - 2\theta^2 + 4\theta - 1)|z| - 2\cos\psi}{(1+\theta^2|z|^2 - 2\theta|z|\cos\psi)^2} \leq 1, \tag{8}$$

Clearly, (8) holds if and only if the numerator in nonnegative, which is certainly true if (7) holds.

Now, we show that (7) is also a necessary condition. Let us substitute $\cos\psi = 0$ in (8). Then

$$|r_\theta(z)|^2 = 1 - |z|\frac{\theta^4|z|^3 + (-2\theta^2 + 4\theta - 1)|z|}{(1+\theta^2|z|^2)^2} \leq 1,$$

for all $z = ir,\ r \in \mathbb{R}$, which is true if and only if

$$-2\theta^2 + 4\theta - 1 \geq 0, \tag{9}$$

which is equivalent to (7). ■

3 Lower bound of the stability constant

In this section we give a lower bound for C_θ when θ ranges within the A-stability bounds (7). First, note that $C_\theta \geq 1$. To see this, first observe that $\tau Ae = 0$ for $e = (...,1,1,1,...)^\top$. Therefore 0 is an eigenvalue of τA with eigenvector e. Since τA is a bounded operator and r_θ is a rational function, the spectral mapping theorem holds [1]. Thus, $r_\theta(0) = 1$ is an eigenvalue of $r_\theta(\tau A)$ with an eigenvector e, i.e., $r_\theta(\tau A)e = e$. Hence, $C_\theta \geq ||r_\theta(\tau A)e||_\infty = 1$. This, together with (5), implies that if $\theta \in [\frac{1}{3}, 1]$ then $C_\theta = 1$.

Now, we compute the exact value $||r_\theta(\tau A)||_\infty$ for $\theta \in (0, \frac{1}{3})$ and $\theta > 1$. Clearly, $||r_\theta(\tau A)||_\infty$ is a lower bound for C_θ for all $\tau > 0$ and $h > 0$. Let $\mu := \frac{\tau}{h^2}$. In [6] it is shown that if the function $f(z) := r_\theta(\mu(z^{-1} - 2 + z))$ has the Laurent expansion $f(z) = \sum_{n=-\infty}^{\infty} \gamma_n z^n$, then $||r_\theta(\tau A)||_\infty = \sum_{n=-\infty}^{\infty} |\gamma_n|$. There it is also shown that the Laurent coefficients for the RDA method are of the form

$$\gamma_k = \gamma_{-k} = \frac{\omega^k(1-\omega)}{\theta(1+\omega)^3}[\omega(\mu^{-1} + 6\theta - 2) + (1-\theta)(1-\omega^2)k], \; k \geq 0, \quad (10)$$

where

$$\omega = \frac{2 + \frac{1}{\theta\mu} - \sqrt{(2 + \frac{1}{\theta\mu})^2 - 4}}{2}.$$

Theorem 3.1 *If $\theta \in (0, \frac{1}{3})$, then*

$$\begin{aligned} ||r_\theta(\tau A)||_\infty &= \frac{\omega(\omega-1)}{\theta(1+\omega)^3}(\mu^{-1} + 6\theta - 2) + \\ 2(a\omega\frac{2\omega^N - 1}{\omega - 1} &+ b\omega\frac{2N\omega^{N+1} - 2(N+1)\omega^N + 1}{(\omega-1)^2}) \end{aligned} \quad (11)$$

if $\mu > (2 - 6\theta)^{-1}$, where

$$a = \frac{\omega - 1}{\theta(1+\omega)^3}(\omega(\mu^{-1} + 6\theta - 2)), \; b = \frac{\omega - 1}{\theta(1+\omega)^3}(1-\theta)(1-\omega^2) \quad (12)$$

and

$$N = [\frac{\omega(\mu^{-1} + 6\theta - 2)}{(\theta - 1)(1-\omega^2)}]. \quad (13)$$

If $0 < \mu \leq (2 - 6\theta)^{-1}$, then $||r_\theta(\tau A)||_\infty = 1$.

Proof. By (6) we only have to prove (11). Let $\mu > (2-6\theta)^{-1}$ be fixed. Then, for $k \le N$, where N is defined in (13), from (10) we have

$$\begin{aligned} |\gamma_k| = |\gamma_{-k}| &= \frac{\omega^k(1-\omega)}{\theta(1+\omega)^3}[-\omega(\mu^{-1}+6\theta-2)-(1-\theta)(1-\omega^2)k] \quad (14) \\ &= a\omega^k + b\omega^k k, \end{aligned}$$

where a and b are defined in (12). If $k > N$ then

$$|\gamma_k| = |\gamma_{-k}| = -a\omega^k - b\omega^k k.$$

Therefore, we have

$$\begin{aligned} ||r_\theta(\tau A)||_\infty = |\gamma_0| + 2\sum_{k=1}^{\infty}|\gamma_k| &= |\gamma_0| + 2\{\sum_{k=1}^{N}(a\omega^k + b\omega^k k) \\ + \sum_{k=N+1}^{\infty}(-a\omega^k - b\omega^k k)\} &= |\gamma_0| + 2\{2(\sum_{k=1}^{N}(a\omega^k + b\omega^k k) \\ &+ \sum_{k=1}^{\infty}(a\omega^k + b\omega^k k)\}. \end{aligned}$$

Finally, since

$$\sum_{k=1}^{N}(a\omega^k + b\omega^k k) = a\omega\frac{\omega^N - 1}{\omega - 1} + b\omega\frac{N\omega^{N+1} - (N+1)\omega^N + 1}{(\omega-1)^2})$$

and

$$\sum_{k=1}^{\infty}(a\omega^k + b\omega^k k) = a\omega\frac{1}{1-\omega} + b\omega\frac{1}{(1-\omega)^2}$$

using (14) for $k = 0$ we get (11). ∎

Similarly for $\theta > 1$, one can prove the following theorem.

Theorem 3.2 *If $\theta > 1$, then for all $\tau, h > 0$ we have*

$$\begin{aligned} ||r_\theta(\tau A)||_\infty &= \frac{\omega(1-\omega)}{\theta(1+\omega)^3}(\mu^{-1}+6\theta-2) + \\ 2(a\omega\frac{2\omega^N - 1}{\omega - 1} &+ b\omega\frac{2N\omega^{N+1} - 2(N+1)\omega^N + 1}{(\omega-1)^2}), \end{aligned}$$

where

$$a = \frac{1-\omega}{\theta(1+\omega)^3}(\omega(\mu^{-1}+6\theta-2)),\ \ b = \frac{1-\omega}{\theta(1+\omega)^3}(1-\theta)(1-\omega^2)$$

and

$$N = [\frac{\omega(\mu^{-1}+6\theta-2)}{(\theta-1)(1-\omega^2)}].\ \blacksquare$$

Note, that in Theorem 3.1 and in Theorem 3.2 the value of N depends on the value of μ. Therefore, if we want to compute the norm $||r_\theta(\tau A)||_\infty$, first we have to choose a value for τ and h. For $\theta = 1 - \frac{1}{2}\sqrt{2}$ we found that for $||r_\theta(\tau A)||_\infty = 1,066$ at $\mu = 15$. As we mentioned in the beginning of this section this is a lower bound of the stability constant $C_{1-\frac{1}{2}\sqrt{2}}$.

4 Upper bound of the stability constant

In this section, using the resolvent estimate (2), first we give an upper bound for $||r_\theta^n(\tau A)||_\infty$ uniform in n. The basis for our calculation is the Dunford-Scwartz representation

$$r_\theta(\tau A)^n = r_\theta(\infty)^n + \frac{1}{2\pi i}\int_\Gamma r_\theta^n(z)R(z,\tau A)\mathrm{d}z, \tag{15}$$

where $\Gamma = \gamma_{\frac{\varepsilon}{n}} \cup \Gamma_{\frac{\varepsilon}{n}}^{\rho_\theta} \cup \gamma_{\rho_\theta}$ with $\gamma_{\frac{\varepsilon}{n}} = \{z; |z| = \frac{\varepsilon}{n},\ -\psi \le \arg(z) \le \psi\}$, $\Gamma_{\frac{\varepsilon}{n}}^{\rho_\theta} = \{z; \frac{\varepsilon}{n} \le |z| \le \rho_\theta,\ \arg(z) = \psi,\ \arg(z) = -\psi\}$ and $\gamma_{\rho_\theta} = \{z; |z| = \rho_\theta,\ -\psi \le \arg(z) \le \psi\}$. Here $0 < \varepsilon < \frac{1}{\theta}$, $\frac{\pi}{2} < \psi < \pi$ are arbitrary and ρ_θ is a number with $|r_\theta(\rho_\theta)| \le 1$. Note that since $r_\theta(\infty) = 0$ the first term turns into 0 in the sum in (15). The idea of using the Dunford-Schwartz representation of the approximating operators in order to estimate the stability constant of the Crank-Nicolson scheme can be found in [4]. However, for the RDA method the estimates are considerably more complicated, and, since $r_\theta(\infty) = 0$, the path of integration is also different.

Lemma 4.1 *For* $|z| = \frac{\varepsilon}{n} > \frac{1}{\theta}$ *the inequality*

$$|r_\theta^n(z)| \le \frac{1}{1-\theta\varepsilon}\exp(\frac{\varepsilon(1+\theta)}{1-\theta\varepsilon}) \tag{16}$$

holds for all $n \ge 1$.

Proof. We can rewrite r_θ as follows

$$r_\theta(z) = \frac{1}{1-\theta z}(1 + z + \frac{\theta z^2 - \theta z}{1-\theta z}).$$

Then for $|z| < \frac{1}{\theta}$ we have

$$|r_\theta(z)| \leq \frac{1}{1-\theta|z|}(1 + |z| + \frac{\theta|z|^2 + \theta|z|}{1-\theta|z|}).$$

Now, using the elementary inequalities $1 \leq 1 + |z| \leq \exp|z|$ we obtain

$$|r_\theta(z)| \leq \frac{1}{1-\theta|z|}\exp|z|(1 + \theta\frac{|z|^2 + |z|}{1-\theta|z|})$$

thus

$$|r_\theta^n(z)| \leq (1-\theta|z|)^{-n}\exp(n|z|)(1 + \theta\frac{|z|^2 + |z|}{1-\theta|z|})^n.$$

Therefore, taking $|z| = \frac{\varepsilon}{n}$ we have

$$|r_\theta^n(z)| \leq (1-\theta\frac{\varepsilon}{n})^{-n}\exp(\varepsilon)(1 + \theta\frac{\varepsilon^2 + n\varepsilon}{n^2 - \theta n\varepsilon})^n.$$

Since the sequence $(1-\theta\frac{\varepsilon}{n})^{-n}$ is monotonically decreasing and clearly $(1 + \frac{1}{x})^x \leq e$ for all $x > 0$, we obtain

$$|r_\theta^n(z)| \leq \frac{1}{1-\theta\varepsilon}\exp(\varepsilon)\exp(\theta\frac{\varepsilon^2 + n\varepsilon}{n-\theta\varepsilon}).$$

Finally,

$$\theta\frac{\varepsilon^2 + n\varepsilon}{n-\theta\varepsilon} = \theta(\frac{\varepsilon^2}{n-\theta\varepsilon} + \varepsilon + \varepsilon\frac{\theta\varepsilon}{n-\theta\varepsilon}) \leq \theta(\frac{\varepsilon^2}{1-\theta\varepsilon} + \varepsilon + \varepsilon\frac{\theta\varepsilon}{1-\theta\varepsilon}),$$

which gives (16). ■

Corollary 4.1 *For all $n \geq 1$ we have*

$$||\frac{1}{2\pi i}\int_{\gamma_{\frac{\varepsilon}{n}}} r_\theta^n(z)R(z,\tau A)\,dz|| \leq \frac{2}{\pi}\frac{1}{1-\theta\varepsilon}\exp(\frac{\varepsilon(1+\theta)}{1-\theta\varepsilon})\ln\tan(\frac{\psi+\pi}{4}).$$

Proof. Using the resolvent estimate (2) and Lemma 4.1 we have

$$||\frac{1}{2\pi i}\int_{\gamma_{\frac{\varepsilon}{n}}} r_\theta^n(z)R(z,\tau A)\mathrm{d}z|| \leq \frac{1}{\pi}\int_0^\psi |r_\theta^n(\frac{\varepsilon}{n}e^{i\phi})|\sec\frac{\phi}{2}\mathrm{d}\phi \leq$$

$$\frac{2}{\pi}\frac{1}{1-\theta\varepsilon}\exp(\frac{\varepsilon(1+\theta)}{1-\theta\varepsilon})\ln\tan(\frac{\psi+\pi}{4}). \blacksquare$$

Proposition 4.1 *For all $n \geq 1$ we have*

$$||\frac{1}{2\pi i}\int_{\gamma_{\rho_\theta}} r_\theta^n(z)R(z,\tau A)\,dz|| \leq \frac{2}{\pi}\ln\tan(\frac{\psi+\pi}{4}). \tag{17}$$

Proof. Since $r_\theta(\infty)=0$, therefore there is a number ρ_θ, such that $r_\theta(\rho_\theta) \leq 1$. Then using again the resolvent estimate (2) we get (17). $\blacksquare$

A lower bound for ρ_θ can be derived from (8). Since for $\theta \in [1-\frac{1}{2}\sqrt{2}, 1+\frac{1}{2}\sqrt{2}]$ the family r_θ is A-stable, it is enough to consider the case when $\cos\psi \in [0,1]$. Therefore ρ_θ can be obtained from the inequality

$$\theta^4\rho_\theta^3 - 4\theta^3\cos\psi\rho_\theta^2 + (4\theta^2\cos^2\psi - 2\theta^2 + 4\theta - 1)\rho_\theta - 2\cos\psi \geq 0,$$

for all $\cos\psi \in [0,1]$. Again, using (7), we arrive at the following sufficient condition

$$\theta^4\rho_\theta^3 - 4\theta^3\rho_\theta^2 - 2 \geq 0.$$

Then a lower bound for ρ_θ can be easily computed. (For example, for $\theta = 1-\frac{1}{2}\sqrt{2}$ we have $\rho_{1-\frac{1}{2}\sqrt{2}} = 14.8837$.)

Let us decompose the path $\Gamma_{\frac{\varepsilon}{n}}^{\rho_\theta} = \Gamma_{\frac{\varepsilon}{n}}^{L} \cup \Gamma_L^{\rho_\theta}$, where $\frac{\varepsilon}{n} < L \leq \rho_\theta$ is arbitrary.

Lemma 4.2 *If $z \in \Gamma_{\frac{\epsilon}{n}}^L$ then*

$$|r_\theta^n(z)| \leq \exp(-\frac{c(\theta,L)}{2}|z|n), \tag{18}$$

where $c(\theta,L) = \frac{-2\cos\psi}{(1+\theta^2L^2-2\theta L\cos\psi)^2}$

Proof. First, note that by (9) the inequality $-2\theta^2+4\theta-1 \geq 0$ holds. Also, if $z \in \Gamma_{\frac{\epsilon}{n}}^L$, then $\cos\arg(z) \leq 0$. Therefore, from (8) it follows, that for $z \in \Gamma_{\frac{\epsilon}{n}}^L$

$$|r_\theta^2(z)| \leq 1 - |z|c(\theta,L),$$

where $c(\theta, L) = \frac{-2\cos\psi}{(1+\theta^2 L^2 - 2\theta L\cos\psi)^2}$. Hence, if $z \in \Gamma^L_{\frac{\epsilon}{n}}$, then

$$|r_\theta^n(z)| \le \exp(-\frac{c(\theta, L)}{2}|z|n). \blacksquare$$

Proposition 4.2 *For all $n \ge 1$ we have*

$$||\frac{1}{2\pi i}\int_{\Gamma^L_{\frac{\varepsilon}{n}}} r_\theta^n(z) R(z, \tau A)\,dz|| \le$$
$$\frac{1}{\pi\cos\frac{\psi}{2}}(-\ln(\frac{c(\theta, L)\varepsilon}{2}) - \gamma \quad + \quad \sum_{s=1}^{2m+1} \frac{(-1)^{s-1}}{s}\frac{(\frac{c(\theta,L)\varepsilon}{2})^s}{s!}), \qquad (19)$$

where $\gamma = 0.57721...$ denotes the Euler constant and $m \in I\!N$ is arbitrary.

Proof. Using (18) we may write

$$||\frac{1}{2\pi i}\int_{\Gamma^L_{\frac{\varepsilon}{n}}} r_\theta^n(z) R(z, \tau A)\mathrm{d}z|| \le$$
$$\frac{1}{\pi}\int_{\frac{\varepsilon}{n}}^{L} \exp(-\frac{c(\theta, L)}{2}tn)\frac{1}{t\cos\frac{\psi}{2}}\ \mathrm{d}t \quad = \quad \frac{1}{\pi\cos\frac{\psi}{2}}\int_{\frac{c(\theta,L)\varepsilon}{2}}^{\frac{c(\theta,L)Ln}{2}} \exp(-s)\frac{1}{s}\ \mathrm{d}s \le$$
$$\frac{1}{\pi\cos\frac{\psi}{2}}\int_{\frac{c(\theta,L)\varepsilon}{2}}^{\infty} \exp(-s)\frac{1}{s}\ \mathrm{d}s.$$

Finally, recalling the formula (see e.g. [5])

$$\int_c^\infty \exp(-s)\frac{1}{s}\ \mathrm{d}s = -\ln c - \gamma + \sum_{k=1}^{\infty}\frac{(-1)^{k-1}}{k}\frac{c^k}{k!},$$

we obtain (19). $\blacksquare$

Proposition 4.3 *For all $n \ge 1$ we have,*

$$||\frac{1}{2\pi i}\int_{\Gamma^{\rho_\theta}_L} r_\theta^n(z) R(z, \tau A)\,dz|| \le \frac{\ln\frac{\rho_\theta}{L}}{\pi\cos\frac{\psi}{2}}.$$

Proof. The resolvent estimate (2) and the A-stability of r_θ yields

$$||\frac{1}{2\pi i}\int_{\Gamma^{\rho_\theta}_L} r_\theta^n(z) R(z, \tau A)\mathrm{d}z|| \le \frac{1}{\pi\cos\frac{\psi}{2}}\int_L^{\rho_\theta}\frac{1}{s}\ \mathrm{d}s = \frac{\ln\frac{\rho_\theta}{L}}{\pi\cos\frac{\psi}{2}}. \blacksquare$$

The upper bound for $||r_\theta^n(\tau A)||_\infty$ can be obtained using Proposition 4.1, Proposition 4.2, Proposition 4.3 and Corollary 4.1 by choosing different values for the arbitrary numbers ε, ψ and L. We choose $m = 3$ in (19). For $\theta = 1 - \frac{1}{2}\sqrt{2}$, using a discrete grid for the possible values of ε, ψ and L with MATLAB 5.3 an upper bound equals 4.0512 for $\varepsilon = 0.2610$, $\psi = 1.7279$ and $L = 3.3780$.

Now, we consider the heat equation on a finite interval with the homogeneous Dirichlet boundary condition

$$\begin{aligned} \frac{\partial u}{\partial t} &= \frac{\partial^2 u}{\partial x^2} \quad x \in [0,1],\ t \geq 0, \\ u(x,0) &= u_0(x),\ x \in [0,1],\ u(0,t) = u(1,t) = 0,\ t \geq 0. \end{aligned}$$

After the discretization the matrix in (1) is here of the form

$$A_s := \frac{1}{h^2}\text{tridiag}[1,-2,1] \in \mathbb{R}^{s\times s},$$

where $h = \frac{1}{s+1}$. As we indicated in the Introduction, the estimate for the stability constant is also valid in this case. The next theorem will show that contrary to the infinite interval case, for τ large enough $||r_\theta^n(\tau A_s)||_\infty < 1$ for all $\theta \in \mathbb{R}$.

Theorem 4.1 *For all $n \geq 1$ and $\theta \in \mathbb{R}$ we have*

$$||r_\theta^n(\tau A_s)||_\infty \leq \\ \left(\frac{1}{1+2\theta\frac{\tau}{h^2}(1-\cos\frac{\pi}{s+1})}\right)^n\left(\left|\frac{2\theta-1}{\theta}\right| + \left|\frac{1-\theta}{\theta}\right|\frac{1}{1+2\theta\frac{\tau}{h^2}(1-\cos\frac{\pi}{s+1})}\right)^n. \quad (20)$$

Proof. The eigenvalues of the matrix A_s are

$$\lambda_s^{(k)} = \frac{2}{h^2}(-1+\cos\frac{k\pi}{s+1}),\ k = 1, ..., s, \quad (21)$$

(see e.g. [8]). Notice, that

$$r_\theta(\tau A_s) = \frac{2\theta-1}{\theta}\frac{1}{\theta\tau}R(\frac{1}{\theta\tau}, A_s) + \frac{1-\theta}{\theta}(\frac{1}{\theta\tau})^2 R^2(\frac{1}{\theta\tau}, A_s).$$

Also, observe that the matrix A_s generates a contraction semigroup in the maximum norm. This follows from the facts that $A_s = \text{tridiag}[1,0,1] - 2I$

and that the matrices tridiag$[1,0,1]$ and $-2I$ commute, hence

$$||\exp(tA_s)||_\infty = ||\exp(t\frac{1}{h^2}\text{tridiag}[1,0,1])\exp(t\frac{1}{h^2}(-2I))||_\infty \leq$$
$$\exp(t\frac{1}{h^2}||\text{tridiag}[1,0,1]||_\infty)\exp(-2t\frac{1}{h^2}) = \exp(2t\frac{1}{h^2})\exp(-2t\frac{1}{h^2}) = 1.$$

Then from the Hille-Yoshida theorem (see e.g. [2]) it follows that

$$||r_\theta^n(\tau A_s)||_\infty \leq (\frac{\frac{1}{\theta\tau}}{\frac{1}{\theta\tau} - \lambda_s^{(1)}})^n(|\frac{2\theta-1}{\theta}| + |\frac{1-\theta}{\theta}|\frac{\frac{1}{\theta\tau}}{\frac{1}{\theta\tau} - \lambda_s^{(1)}})^n. \tag{22}$$

Finally, using (21) with $k = 1$, (22) implies (20). ■

Note that (20) shows that $||r_\theta^n(\tau A_s)||_\infty < 1$ for all $\tau, h > 0$ if $\theta \in [\frac{1}{2}, 1]$. Also, observe that the estimate is not optimal since we already know that $||r_\theta^n(\tau A_s)||_\infty \leq 1$ if $\theta \in [\frac{1}{3}, 1]$. As we have already mentioned, for τ large enough $||r_\theta^n(\tau A_s)||_\infty < 1$ for all $\theta \in \mathbb{R}$. This behavior is different from the infinite interval case and basically follows from the facts that $r_\theta(\infty) = 0$ and that the spectrum of A_s lies strictly on the left axis. This remarkable property allows a much wider choice for the discretization parameters if we want to preserve the conractivity in the maximum norm.

5 Concluding remarks

The method we used allows the analysis of more general cases. The estimations derived for the complex functions $r_\theta(z)$ in Section 4 can be used to obtain stability constants for $r_\theta(\tau A)$ with more general matrices A if the appropriate resolvent estimate is known. Also, the method to obtain the norm estimate in the finite interval case can be generalized to a wider class of matrices, since the computation of the first eigenvalue and the bound of the matrix semigroup in the maximum norm are the essential steps. Finally, we remark that the knowledge of the stability constant can be used to obtain second order unconditionally contractive finite difference methods (see [3]).

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