

A SPECTRAL ORDER METHOD FOR INVERTING SECTORIAL LAPLACE TRANSFORMS

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Abstract. Laplace transforms which admit a holomorphic extension to some sector strictly containing the right half plane and exhibiting a potential behavior are considered. A spectral order, parallelizable method for their numerical inversion is proposed. The method takes into account the available information about the errors arising in the evaluations. Several numerical illustrations are provided.

Key words. Laplace transform, numerical inversion, parabolic, spectral order, parallelizable.

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1. Introduction. In a variety of situations, the problem arises of inverting numerically the Laplace transform $U(z)$ of a given mapping of interest $u(t)$. Roughly speaking, it turns out that the wider the set W where $U(z)$ can be computed is, the easier the inversion results. For instance, if W is an interval (a, b) then the numerical inversion becomes an ill-posed problem [1, 8, 9]. On the other hand, if W is the complement of some bounded region, then the efficient Talbot's method [19, 25] is at hand.

In the present paper we focus on the particular situation where W is a sector symmetric with respect to the real axis, strictly containing the right half plane, and we assume that $U(z)$ exhibits a potential behavior on W . We say then that $U(z)$ is *sectorial*. Precisely, there is a renewed interest in the numerical inversion of *sectorial* mappings [10, 11, 14, 16, 21], mainly due to its applicability to linear, nonhomogeneous evolution equations of parabolic type (both in the context of abstract IVP's and Volterra equations), as well as their discretizations in space [2, 3]. Notice that the applicability of the inversion approach, in the *sectorial* setting, demands in practice that the source term of the parabolic equation must be approximated efficiently (at least locally) by holomorphic mappings [11, 16]. This difficulty is overcome in [12, 20], where the ideas in the present paper are adapted so as to provide accurate reconstructions of the traditional Runge-Kutta approximations to the solutions of such parabolic problems. These reconstructions require no regularity on the source term of the problem.

In the present paper we consider the issue of the numerical inversion of *sectorial* mappings by itself. To fix ideas, let

$$u : (0, +\infty) \rightarrow X$$

be a locally integrable mapping, taking values in a Banach space X , with exponential growth. Denote by

$$U(z) = \int_0^{+\infty} e^{-zt} u(t) dt$$

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its Laplace transform. We will always assume that $U(z)$ admits a holomorphic extension to the complement W of some acute sector

$$\Sigma_\delta = \{z \in \mathbb{C} : |\arg(-z)| \leq \delta\}, \quad 0 < \delta < \frac{\pi}{2}, \quad (1.1)$$

and that there exist constants $M > 0$ and $\mu \in \mathbb{R}$ such that

$$\|U(z)\| \leq \frac{M}{|z|^\mu}, \quad z \notin \Sigma_\delta. \quad (1.2)$$

The last requirement, with $\mu \geq 1$, means that u admits a bounded and holomorphic extension to any sector of the form $|\arg(z)| \leq \delta'$, with $0 < \delta' < \pi/2 - \delta$. If $\mu < 1$, we select an integer number $m \geq 1$, with $m + \mu \geq 1$, and set $V(z) = U(z)/z^m$. Then, by the previous remark, $V(z)$ is the Laplace transform of a mapping $v : (0, +\infty) \rightarrow X$, which admits a bounded and holomorphic extension to sectors with semiangle δ' as before, and now u is understood to be the derivative of order m of v .

Notice that in case $U(z)$ satisfies a similar inequality

$$\|U(z)\| \leq \frac{M}{|z - \omega|^\mu}, \quad z \notin \omega + \Sigma_\delta,$$

for some $\omega \in \mathbb{R}$, then, by using the shifting theorem, the inversion of $U(z)$ is reduced to the one of a Laplace transform $\tilde{U}(z)$ fulfilling (1.2). Since the respective originals $u(t)$ and $\tilde{u}(t)$ are related by $u(t) = e^{\omega t}\tilde{u}(t)$, then we can just approximate $\tilde{u}(t)$. This is why the analysis is restricted to the situation $\omega = 0$, i.e. to (1.2).

The goal is to numerically reconstruct u from knowledge of a moderate number of evaluations of $U(z)$ at suitable nodes $z \notin \Sigma_\delta$. Let us point out that, from a practical point of view, it is essential to take into account that these evaluations are going to be affected by errors.

The starting point of the method we propose is the well-known inversion formula

$$u(t) = \frac{1}{2\pi i} \int_\Gamma e^{tz} U(z) dz, \quad t > 0, \quad (1.3)$$

where Γ is a suitable path connecting $-i\infty$ to $+i\infty$ which, in our setting, can be taken so as to guarantee the absolute convergence of the integral appearing in (1.3). As in [10, 14, 16], we choose Γ the branch of a hyperbola parametrized by a mapping $S : (-\infty, +\infty) \rightarrow \mathbb{C}$ admitting a holomorphic extension to a horizontal strip around the real axis. The numerical method we propose is simply the truncated trapezoidal rule, applied to the definite integral arising after parametrizing (1.3) by S , used with $2n+1$ nodes $x_k = kh$, $-n \leq k \leq n$, and a suitable step size $h > 0$. The properties of S allow us to use the ideas and results in [23, 24], where the trapezoidal rule applied to holomorphic mappings on strips is considered. Let us comment that the fast decay of our integrand [10, 14] yields an improvement of the more general estimates in [23, 24].

Very often, for instance in the context of IVP's (see Illustration 3 in Section 5), the main computational effort of the method is due to the evaluations of $U(z)$ at the nodes $z_k = S(x_k)$, $-n \leq k \leq n$. An important feature of the present approach is that the same evaluations can be used to approximate $u(t)$ at different $t > 0$ [14, 19]. Accordingly, our goal is to obtain a uniform error estimate for the approximation of $u(t)$ on intervals of the form $[t_0, \Lambda t_0]$, with given $t_0 > 0$ and $\Lambda \geq 1$, rather than at a fixed $t > 0$. Essentially, this was the aim in [14], whose basic estimates we

borrow. Notice also that the algorithm presents two levels of parallelism since, first, the evaluations of $U(z)$ at the involved nodes and, second, the evaluations of $u(t)$ at a selected finite set of values of $t \in [t_0, \Lambda t_0]$, can be carried out on different processors.

In the present paper, by considering a different choice of the geometrical and scale parameters from the one in [14], we improve the results there in two different ways:

- (i) We get a better error bound, which now turns out to be a genuine spectral estimate of the form $O(e^{-cn})$.
- (ii) We also get a weaker dependence of the exponential factor c on Λ , since now $c = O(1/\ln \Lambda)$.

This means, in practice, that with a moderate number of evaluations of $U(z)$ we can accurately approximate $u(t)$, uniformly on intervals $[t_0, t_1]$ with $\Lambda = t_1/t_0 \gg 1$, let us say $\Lambda = 50$.

On the other hand, for the choice of parameters we propose, the precision ρ used in the evaluations of $U(z)$ at the required nodes plays a more relevant role than in [14]. In fact, ignoring that we always have $\rho > 0$ would result in large actual errors for $n \gg 1$, as simple numerical experiments show (see Illustration 1 in Section 5). This drawback is overcome by minimizing the estimate we get for the actual error (Theorem 2), which leads to a (ρ, n) -dependent choice of parameters. With this choice, the actual error finally behaves for moderate n like $O(e^{-cn})$, with $c = O(1/\ln \Lambda)$, and for large n like $O(\rho)$. This optimal choice of parameters demands, of course, some information about the size of ρ . In the absence of it, we propose an n -dependent choice of parameters for which the actual error behaves like $O(\rho + e^{-cn})$, with $c = O(1/(\ln n + \ln \Lambda))$. All the above estimates are uniform on $t_0 \leq t \leq \Lambda t_0$, with fixed $t_0 > 0$ and $\Lambda > 1$. Moreover, the error constants are made explicit in the analysis and turn out to be reasonable.

The outline of the paper is as follows. In Section 2 we describe the numerical method and show, in Theorem 1, how to achieve (i) and (ii). The propagation of errors is studied in Section 3. The choice of parameters is considered in Section 4 and four simple numerical illustrations of the theoretical results are provided in Section 5.

2. The numerical method. Given δ in (1.1) and following the ideas in [14], we select $\alpha, d > 0$ such that

$$0 < \alpha - d < \alpha + d < \frac{\pi}{2} - \delta. \quad (2.1)$$

Defining

$$T(w) = 1 - \sin(\alpha + iw) \quad (2.2)$$

this mapping transforms each horizontal straight line $\text{Im } w = y$, $-d \leq y \leq d$, into the left branch of the hyperbola given by

$$\left(\frac{\text{Re } z - 1}{\sin(\alpha - y)} \right)^2 - \left(\frac{\text{Im } z}{\cos(\alpha - y)} \right)^2 = 1, \quad (2.3)$$

with center at $(1, 0)$, foci at $(0, 0)$ and $(2, 0)$, whose asymptotes make angles $\pm[\pi/2 - (\alpha - y)]$ with the real axis. Therefore, T transforms the horizontal strip

$$D_d = \{z \in \mathbb{C} : |\text{Im } z| \leq d\}$$

into the region in the complex plane limited by the left branches corresponding to $y = \pm d$ in (2.3).

Introducing a parameter $\lambda > 0$, the parametrization of Γ in (1.3) can be defined as

$$\Gamma = \{\lambda T(x) : x \in \mathbb{R}\},$$

i.e. Γ is the branch of a hyperbola corresponding to the image of the real axis under $S = \lambda T$. This results in

$$u(t) = \int_{-\infty}^{+\infty} G_t(x) dx, \quad t > 0,$$

where $G_t : D_d \rightarrow X$, $t > 0$, is the mapping

$$G_t(w) = -\frac{\lambda}{2\pi i} \exp(\lambda t T(w)) U(\lambda T(w)) T'(w).$$

Once the parameters α , d , and λ have been fixed, we set $x_k = kh$, $k \in \mathbb{Z}$, and consider the approximation to $u(t)$ given by

$$u_n(t) = h \sum_{k=-n}^n G_t(x_k), \quad t > 0. \quad (2.4)$$

The proof of the main result in [14] (Theorem 2), shows that for $\mu = 1$ in (1.2)

$$\|u(t) - u_n(t)\| \leq M \cdot \varphi(\alpha, d) \cdot L(\lambda t \sin(\alpha - d)) \cdot e^{\lambda t} \left(\frac{1}{e^{2\pi d/h} - 1} + \frac{1}{e^{\lambda t \sin \alpha} \cosh(nh)} \right), \quad (2.5)$$

where

$$\varphi(\alpha, d) = \frac{2}{\pi} \sqrt{\frac{1 + \sin(\alpha + d)}{1 - \sin(\alpha + d)}},$$

and $L(x)$, $x > 0$, is the function

$$L(x) = 1 + |\ln(1 - e^{-x})|.$$

Notice that $L(x)$ is decreasing in x , $L(x) \approx |\ln x|$, for $x \rightarrow 0^+$ and $L(x)$ tends to 1, for $x \rightarrow +\infty$.

As we commented in the Introduction, in many applications the computational effort to obtain $u_n(t)$ is mainly due to the evaluations of $U(z)$ at $z = \lambda T(x_k)$, $-n \leq k \leq n$, but these evaluations could be carried out in parallel. Another attractive feature of (2.4) is that the same evaluations of $U(z)$ can be used to compute $u_n(t)$ for different $t > 0$. In fact, as we see below, with the appropriate choice of parameters, we can use the same evaluations of $U(z)$ so as to have a spectral estimate

$$\|u(t) - u_n(t)\| = \mathcal{O}(e^{-cn}),$$

uniform on intervals $t_0 \leq t \leq t_1$. The exponential factor c turns out to depend weakly on the ratio $\Lambda = t_1/t_0$, given that $c = \mathcal{O}(1/\ln \Lambda)$.

For simplicity the next theorem is restricted to the situation $\mu = 1$ in (1.2). The cases $\mu > 1$ and $\mu < 1$ are treated in subsequent remarks.

THEOREM 1. *Assume that U satisfies (1.2) with $\mu = 1$. Fixing α and d according to (2.1), for $t_0 > 0$, $\Lambda \geq 1$, $0 < \theta < 1$ and $n \geq 1$, the following choice of parameters*

$$h = \frac{1}{n} a(\theta), \quad \lambda = \frac{2\pi d n (1 - \theta)}{t_0 \Lambda a(\theta)}, \quad (2.6)$$

with

$$a(\theta) = \operatorname{arccosh}\left(\frac{\Lambda}{(1-\theta)\sin\alpha}\right),$$

yields the uniform estimate on $t_0 \leq t \leq \Lambda t_0$

$$\|u(t) - u_n(t)\| \leq M \cdot \varphi(\alpha, d) \cdot L(\lambda t_0 \sin(\alpha - d)) \cdot \frac{2\epsilon_n(\theta)^\theta}{1 - \epsilon_n(\theta)}, \quad (2.7)$$

where

$$\epsilon_n(\theta) = \exp\left(-\frac{2\pi d}{a(\theta)}n\right).$$

The theorem shows, just by selecting any $0 < \theta < 1$, a genuine spectral order of convergence in n of the form $O(e^{-cn})$, where $c = O(1/\ln \Lambda)$ (cf. [10, 14]).

Proof. Set $\sigma = \lambda t_0$. For $t_0 \leq t \leq \Lambda t_0$, (2.5) implies the uniform bound

$$\|u(t) - u_n(t)\| \leq M \cdot \varphi(\alpha, d) \cdot L(\sigma \sin(\alpha - d)) \cdot e^{\Lambda\sigma} \left(\frac{1}{e^{2\pi d/h} - 1} + \frac{1}{e^{\sigma \sin \alpha \cosh(nh)}} \right).$$

Our choice of h and λ is precisely the one guaranteeing that

$$\exp\left(\frac{2\pi d}{h}\right) = \exp(\sigma \sin \alpha \cosh(nh)) = \frac{1}{\epsilon_n(\theta)},$$

hence

$$\frac{1}{e^{2\pi d/h} - 1} + \frac{1}{e^{\sigma \sin \alpha \cosh(nh)}} \leq \frac{2e^{-2\pi d/h}}{1 - e^{-2\pi d/h}} = \frac{2\epsilon_n(\theta)}{1 - \epsilon_n(\theta)}.$$

The proof ends after remarking that

$$e^{\Lambda\sigma} \epsilon_n(\theta) = \epsilon_n(\theta)^{\theta-1} \epsilon_n(\theta) = \epsilon_n(\theta)^\theta. \quad \square$$

To end the section we comment, in the two following remarks, on the situation $\mu \neq 1$ in (1.2). We omit details in the proofs, which are completely analogous to the one of Theorem 1.

REMARK 1. Assume that U satisfies (1.2) with $\mu > 1$. By Remark 1 in [14] we have

$$\|u(t) - u_n(t)\| \leq M \cdot \varphi(\alpha, d, \mu) \cdot L(\lambda t \sin(\alpha - d)) \cdot \frac{e^{\lambda t}}{\lambda^{\mu-1}} \left(\frac{1}{e^{2\pi d/h} - 1} + \frac{1}{e^{\lambda t \sin \alpha \cosh(nh)}} \right),$$

where

$$\varphi(\alpha, d, \mu) = \frac{2}{\pi} \sqrt{\frac{1 + \sin(\alpha + d)}{(1 - \sin(\alpha + d))^{2\mu-1}}}.$$

Thus, for $0 < \theta < 1$, the same choice of values for h and λ as in Theorem 1 gives the bound

$$\|u(t) - u_n(t)\| \leq M \cdot \varphi(\alpha, d, \mu) \cdot L(\lambda t_0 \sin(\alpha - d)) \cdot \lambda^{1-\mu} \cdot \frac{2\epsilon_n(\theta)^\theta}{1 - \epsilon_n(\theta)},$$

uniformly for $t_0 \leq t \leq \Lambda t_0$. This estimate is again spectral in n , since

$$\lambda^{1-\mu} = O\left(\left(\frac{\Lambda t_0}{n}\right)^{\mu-1}\right).$$

REMARK 2. Assume now that U satisfies (1.2) with $\mu < 1$. By Remark 1 in [14], for a fixed $s \in (0, 1)$, there holds

$$\|u(t) - u_n(t)\| \leq M \cdot \varphi_s(\alpha, d, \mu) \cdot L(s\lambda t \sin(\alpha - d)) \cdot \frac{e^{\lambda t}}{t^{1-\mu}} \left(\frac{1}{e^{2\pi d/h} - 1} + \frac{1}{e^{s\lambda t \sin \alpha \cosh(nh)}} \right),$$

where now

$$\varphi_s(\alpha, d, \mu) = \frac{2}{\pi} \sqrt{\frac{1 + \sin(\alpha + d)}{1 - \sin(\alpha + d)}} \left(\frac{1 - \mu}{(1 - s)e \sin(\alpha - d)} \right)^{1-\mu}.$$

In this situation, for $\theta \in (0, 1)$ we choose

$$h = \frac{1}{n} a_s(\theta), \quad \lambda = \frac{2\pi d n (1 - \theta)}{t_0 \Lambda a_s(\theta)},$$

where

$$a_s(\theta) = \operatorname{arccosh}\left(\frac{\Lambda}{s(1 - \theta) \sin \alpha}\right).$$

Setting

$$\epsilon_{s,n}(\theta) = \exp\left(\frac{-2\pi d n}{a_s(\theta)}\right),$$

we get the spectral estimate

$$\|u(t) - u_n(t)\| \leq M \cdot \varphi_s(\alpha, d, \mu) \cdot L(s\lambda t_0 \sin(\alpha - d)) \cdot t_0^{\mu-1} \frac{2\epsilon_{s,n}(\theta)^\theta}{1 - \epsilon_{s,n}(\theta)},$$

uniformly for $t_0 \leq t \leq \Lambda t_0$.

3. Error propagation. Numerical experiments (see Section 5), show that for large values of n the estimate (2.7) is not longer true in practice. The explanation of this apparently contradictory behavior lays in the influence of the errors when evaluating U and the elementary functions involved. For the sake of simplicity, we consider first the case $\mu = 1$ in (1.2). The situations $\mu > 1$ and $\mu < 1$ are considered in subsequent remarks.

Let $z_k = \lambda T(x_k)$, $-n \leq k \leq n$, be the nodes used in (2.4). Clearly, in practice, as numerical approximation to $u(t)$ we actually obtain

$$\bar{u}_n(t) = \sum_{k=-n}^n \omega_k(t) U_k, \tag{3.1}$$

where, for $-n \leq k \leq n$, $\omega_k(t) \in \mathbb{C}$ and $U_k \in X$, are approximations to

$$-\frac{\lambda h}{2\pi i} \exp(\lambda t z_k) T'(x_k),$$

and $U(z_k)$, respectively.

To estimate the actual error $\|u(t) - \bar{u}_n(t)\|$ we need to make some assumptions on the approximations used. To this end, we are going to focus on two frequent possibilities, depending on whether we have information on absolute or relative errors due to the evaluations. To be precise, we are going to assume that there exists $\rho > 0$ such that, simultaneously for all $-n \leq k \leq n$, we have either

$$\|U(z_k) - U_k\| \leq \rho \quad \text{and} \quad \omega_k(t) = -\frac{\lambda h}{2\pi i} \exp(\lambda t z_k) T'(x_k) \quad (3.2)$$

or

$$\|\exp(\lambda t z_k) T'(x_k) U(z_k) - \omega_k(t) U_k\| \leq \rho \|\exp(\lambda t z_k) T'(x_k) U(z_k)\|. \quad (3.3)$$

Situation (3.2) arises for instance when $U_k \approx U(z_k)$ are provided by means of some auxiliary routine, let us say by solving a linear system, with prescribed accuracy ρ and moreover the errors due to the evaluations of the elementary functions involved turn out to be negligible compared to ρ . Situation (3.3) is typical when $U(z)$ is an elementary function.

The next theorem yields an estimate of the actual error for these situations. We maintain the notation introduced in Theorem 1.

THEOREM 2. *Assume that U satisfies (1.2) with $\mu = 1$. Fix α, d according to (2.1). For $t_0 > 0$, $\Lambda \geq 1$, $0 < \theta < 1$ and $n \geq 1$, select the parameters*

$$h = \frac{1}{n} a(\theta), \quad \lambda = \frac{2\pi d n (1 - \theta)}{t_0 \Lambda a(\theta)}.$$

Assume also that $\omega_k(t) \in \mathbb{C}$, $t_0 \leq t \leq t_1$, $U_k \in X$, $-n \leq k \leq n$, satisfy either (3.2) or (3.3). Then, the actual error is estimated by

$$\|u(t) - \bar{u}_n(t)\| \leq M \cdot \Phi \cdot Q \cdot \left(\varepsilon \varepsilon_n(\theta)^{\theta-1} + \frac{\varepsilon_n(\theta)^\theta}{1 - \varepsilon_n(\theta)} \right), \quad (3.4)$$

uniformly on $t_0 \leq t \leq \Lambda t_0$, where either

(a) $\varepsilon = \rho / (M t_0)$,

$$\Phi = \max \left\{ \frac{2}{\pi} \sqrt{\frac{1 + \sin(\alpha + d)}{1 - \sin(\alpha + d)}}, \frac{1}{\pi e \sin \alpha} \right\}$$

and

$$Q = \max \left\{ 2L(\lambda t_0 \sin(\alpha - d)), \frac{\ln n}{\ln n - 1} \left[\frac{\ln n}{2n} + L \left(\frac{\lambda t_0 \sin \alpha}{\ln n} \right) \right] \right\}$$

in case (3.2) holds, or

(b) $\varepsilon = \rho$,

$$\Phi = \frac{2}{\pi} \sqrt{\frac{1 + \sin(\alpha + d)}{1 - \sin(\alpha + d)}}$$

and

$$Q = \max\{2L(\lambda t_0 \sin(\alpha - d)), 1/2(h + L(\lambda t_0 \sin \alpha))\},$$

in case (3.3) holds.

Notice that Q depends logarithmically on α , d , $1 - \theta$ and Λ .

The estimate (3.4) given by the theorem, with a fixed $0 < \theta < 1$, shows again a spectral order of convergence $O(e^{-cn})$, with $c = O(1/\ln \Lambda)$, but only for moderate n , to be more precise, as long as $\epsilon_n(\theta) \geq \varepsilon$. In fact, for fixed θ , (3.4) goes to $+\infty$ as $n \rightarrow +\infty$. However, this apparent drawback is overcome by selecting θ in a suitable way, as we explain in Section 4.

Proof. By writing

$$\|u(t) - \bar{u}_n(t)\| \leq \|u(t) - u_n(t)\| + \|u_n(t) - \bar{u}_n(t)\|,$$

and noticing that, for the corresponding Q , (2.7) implies

$$\|u(t) - u_n(t)\| \leq M \cdot \Phi \cdot Q \frac{\epsilon_n(\theta)^\theta}{1 - \epsilon_n(\theta)},$$

the proof is reduced to show that

$$\|u_n(t) - \bar{u}_n(t)\| \leq M \cdot \Phi \cdot Q \varepsilon \epsilon_n(\theta)^{\theta-1}. \quad (3.5)$$

Assume first that (3.2) holds. This situation was already studied in [14], where it was proved that

$$\|u_n(t) - \bar{u}_n(t)\| \leq \frac{\rho \ln n}{2\pi e(\ln n - 1) \sin \alpha} \frac{e^{\lambda t}}{t} \left[\frac{\ln n}{n} + 2L \left(\frac{\lambda t \sin \alpha}{\ln n} \right) \right], \quad (3.6)$$

whence, after recalling that $\varepsilon = \rho/(t_0 M)$ and noticing that

$$e^{\Lambda \lambda t_0} = \epsilon_n(\theta)^{\theta-1}, \quad (3.7)$$

we readily obtain (3.5).

Assume now that (3.3) holds. Proceeding as in the proof of Lemma 1 and Theorem 2 in [14], and denoting

$$\varphi(\alpha, 0) = \frac{2}{\pi} \sqrt{\frac{1 + \sin \alpha}{1 - \sin \alpha}},$$

we get

$$\begin{aligned} \|u_n(t) - \bar{u}_n(t)\| &\leq \frac{\rho M e^{\lambda t}}{2\pi} h \sum_{k=-n}^n e^{-\lambda t \sin \alpha \cosh x_k} \left| \frac{T'(x_k)}{T(x_k)} \right| \\ &\leq \frac{M \varphi(\alpha, 0)}{4} \rho e^{\lambda t} h \sum_{k=-n}^n e^{-\lambda t \sin \alpha \cosh x_k} \\ &\leq \frac{M \varphi(\alpha, 0)}{2} \rho e^{\lambda t} \left(h + \int_0^{+\infty} e^{-\lambda t \sin \alpha \cosh x} dx \right) \\ &\leq \frac{M \varphi(\alpha, 0)}{2} \rho e^{\lambda t} (h + L(\lambda t \sin \alpha)). \end{aligned}$$

Hence, using again (3.7) and the inequality $\varphi(\alpha, 0) \leq \varphi(\alpha, d)$, we deduce (3.5). \square

The behavior $\mu \neq 1$ in (1.2) is considered in the following remarks, whose proofs are a combination of Remark 1, Remark 2 and the arguments used in the proof of Theorem 2 in [14]. Notice that (3.6) is independent of μ .

REMARK 3. Assume that $\mu > 1$ in (1.2) and fix $0 < \theta < 1$. Then, for the choice of parameters in Theorem 2 and uniformly on $t_0 \leq t \leq \Lambda t_0$, we have:

(a) in case (3.2) holds

$$\|u(t) - \bar{u}_n(t)\| \leq M \cdot \Phi \cdot Q \cdot \left(\varepsilon \varepsilon_n(\theta)^{\theta-1} + \lambda^{1-\mu} \frac{\varepsilon_n(\theta)^\theta}{1 - \varepsilon_n(\theta)} \right)$$

with $\varepsilon = \rho/(Mt_0)$,

$$\Phi = \max \left\{ \frac{2}{\pi} \sqrt{\frac{1 + \sin(\alpha + d)}{(1 - \sin(\alpha + d))^{2\mu-1}}}, \frac{1}{\pi e \sin \alpha} \right\}$$

and

$$Q = \max \left\{ 2L(\lambda t_0 \sin(\alpha - d)), \frac{\ln n}{\ln n - 1} \left[\frac{\ln n}{2n} + L \left(\frac{\lambda t_0 \sin \alpha}{\ln n} \right) \right] \right\},$$

(b) in case (3.3) holds

$$\|u(t) - \bar{u}_n(t)\| \leq M \cdot \Phi \cdot Q \cdot \lambda^{1-\mu} \cdot \left(\varepsilon \varepsilon_n(\theta)^{\theta-1} + \frac{\varepsilon_n(\theta)^\theta}{1 - \varepsilon_n(\theta)} \right),$$

with $\varepsilon = \rho$,

$$\Phi = \frac{2}{\pi} \sqrt{\frac{1 + \sin(\alpha + d)}{(1 - \sin(\alpha + d))^{2\mu-1}}}$$

and

$$Q = \max\{2L(\lambda t_0 \sin(\alpha - d)), 1/2(h + L(\lambda t_0 \sin \alpha))\}.$$

REMARK 4. Assume that $\mu < 1$ in (1.2) and fix $0 < s, \theta < 1$. Then, for the choice of parameters in Remark 2 and uniformly on $t_0 \leq t \leq \Lambda t_0$, we have:

(a) in case (3.2) holds

$$\|u(t) - \bar{u}_n(t)\| \leq M \cdot \Phi \cdot Q \cdot \left(\varepsilon \varepsilon_{s,n}(\theta)^{\theta-1} + t_0^{\mu-1} \frac{\varepsilon_{s,n}(\theta)^\theta}{1 - \varepsilon_{s,n}(\theta)} \right),$$

with $\varepsilon = \rho/(Mt_0)$,

$$\Phi = \max \left\{ \frac{2}{\pi} \sqrt{\frac{1 + \sin(\alpha + d)}{1 - \sin(\alpha + d)}} \left(\frac{1 - \mu}{(1 - s)e \sin(\alpha - d)} \right)^{1-\mu}, \frac{1}{\pi e \sin \alpha} \right\}$$

and

$$Q = \max \left\{ 2L(s\lambda t_0 \sin(\alpha - d)), \frac{\ln n}{\ln n - 1} \left[\frac{\ln n}{2n} + L \left(\frac{\lambda t_0 \sin \alpha}{\ln n} \right) \right] \right\},$$

(b) in case (3.3) holds

$$\|u(t) - \bar{u}_n(t)\| \leq M \cdot \Phi \cdot Q \cdot \left(\lambda^{1-\mu} \varepsilon \varepsilon_{s,n}(\theta)^{\theta-1} + t_0^{\mu-1} \frac{\varepsilon_{s,n}(\theta)^\theta}{1 - \varepsilon_{s,n}(\theta)} \right),$$

with $\varepsilon = \rho$,

$$\Phi = \frac{2}{\pi} \sqrt{\frac{1 + \sin(\alpha + d)}{1 - \sin(\alpha + d)}} \left(\frac{1 - \mu}{(1 - s)e \sin(\alpha - d)} \right)^{1-\mu},$$

and

$$Q = \max\{2L(s\lambda t_0 \sin(\alpha - d)), 1/2(h + L(s\lambda t_0 \sin \alpha))\}.$$

4. The choice of parameters. With Theorem 2 in mind, we now try to derive a strategy for the choice of parameters. First of all, (3.4) shows that it is of interest to select α away from zero and $\alpha + d$ away from $\pi/2$. The dependence of the actual error on $\alpha - d$ is less important, since it is logarithmic.

Suppose α and d have been already chosen, then for a given n we take h and λ as indicated in Theorem 2 and we fix $0 < \theta < 1$. Assume also that we have an estimation of ρ and set $\varepsilon = \rho/(Mt_0)$ or $\varepsilon = \rho$ as in Theorem 2. Then, since in practice we always have $\rho > 0$ and hence $\varepsilon > 0$, it turns out that $\varepsilon\epsilon_n(\theta)^{\theta-1} \rightarrow +\infty$, as $n \rightarrow +\infty$. Hence, it is clear that increasing the number of nodes might result in a worse estimate (3.4). In fact, increasing n may result in worse approximations, as Illustration 1 in Section 5 shows.

To overcome this drawback we let θ be a free parameter for the moment. Given $\varepsilon > 0$ and n , after selecting α and d , neglecting the logarithmic factor Q and taking into account that typically $\epsilon_n(\theta) \ll 1$, the best thing we can do is to choose $0 < \theta < 1$ so as to minimize the term

$$\varepsilon\epsilon_n(\theta)^{\theta-1} + \epsilon_n(\theta)^\theta, \quad (4.1)$$

i.e. we must tune θ depending on $\varepsilon > 0$ and n . By a direct calculation it can be proven that the first derivative of $\epsilon_n(\theta)^{\theta-1}$ with respect to θ is increasing in θ . The same is true for $\epsilon_n(\theta)^\theta$ (in this case the proof, though elementary, is more difficult). We conclude that the expression in (4.1) is a convex function of θ . Moreover, its limit either for $\theta \rightarrow 0+$ or $\theta \rightarrow 1-$ is $+\infty$. Therefore, (4.1) attains its minimum exactly for one value $\theta_{\varepsilon,n} \in (0, 1)$, which is the one we propose to be used. Though it is not easy to express the dependence of $\theta_{\varepsilon,n}$ on n and ε , this can be easily done numerically (see Section 5).

Since, up to logarithmic factors, the choice $\theta = \theta_{\varepsilon,n}$ in (3.4) is optimal, it is clear that with this choice we get for the actual error:

- (a) A spectral order of convergence $O(e^{-cn})$ with $c = O(1/\ln \Lambda)$, for moderate values of n , since this is true for any value $0 < \theta < 1$.
- (b) The errors are not propagated. In fact, already with the non-optimal choice

$$\theta = 1 - \frac{1}{n},$$

(3.4) reads

$$\|u(t) - \bar{u}_n(t)\| = O(\varepsilon + e^{-cn}), \quad (4.2)$$

uniformly on $t_0 \leq t \leq \Lambda t_0$, with $c = O(1/(\ln \Lambda + \ln n))$. This remark tells us that, for large values of n , the actual error saturates at level ε , as observed in the numerical experiments (see Section 5).

In the previous discussion it was essential to assume that we had some information about ε . Notice that, even in case we do not have such an information, the choice $\theta = 1 - 1/n$, which led to (4.2), is always available. This bound is almost spectral in n , depends weakly on Λ and prevents error amplification.

5. Numerical illustrations. In this section we give four numerical illustrations. The first two ones concern elementary Laplace transforms which are assumed to be computed with a relative error of order $\rho \approx \text{eps}$, where eps stands for the machine precision ($\text{eps} = 10^{-16}$ in our computations). In the last two illustrations we do not

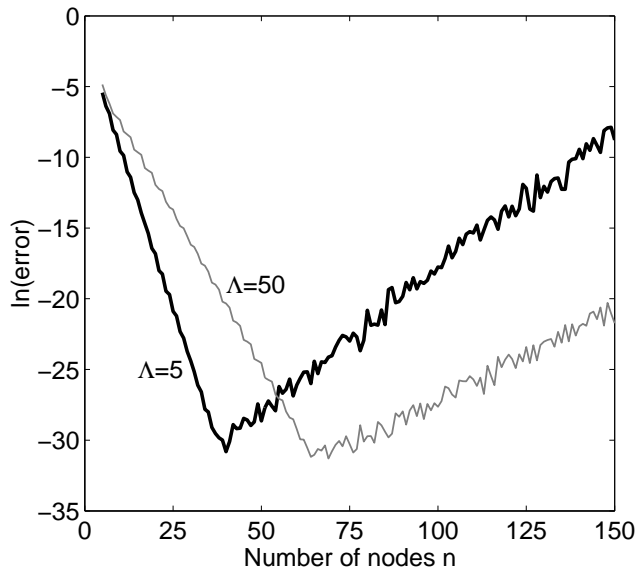


FIG. 5.1. $\ln \max_{t \in [t_0, \Lambda t_0]} \|u(t) - \bar{u}_n(t)\|$ versus n for u in Illustration 1, with $\theta = 0.5$ fixed, $\alpha = 0.7$, $d = 0.6$ and $t_0 = 1$. The gray line corresponds to $\Lambda = 50$ and the black one to $\Lambda = 5$.

assume any information about the errors due to the computations of the Laplace transforms.

ILLUSTRATION 1. We first show by means of a simple example, that for $n \gg 1$ (2.7) fails in the presence of errors in the evaluations. To this end, we consider the mapping $u(t) = e^{-t}$, whose Laplace transform is $U(z) = 1/(1+z)$.

This function satisfies (1.2) for all $\delta > 0$ and $M = 1/\sin \delta$. We fix $\theta = 0.5$, $\alpha = 0.7$, $d = 0.6$ and choose the parameters h , λ as stated in the theorem for all the values of n . In Fig. 5.1 we plot in a semilogarithmic scale the absolute actual error, i.e.

$$\ln \max_{t \in [t_0, \Lambda t_0]} \|u(t) - \bar{u}_n(t)\|$$

versus n (recall that $\bar{u}_n(t)$ stands for the actual computed approximation to $u(t)$, see (3.1)). This is done for $\Lambda = 5, 50$ and $t_0 = 1$. This figure shows that the error decays exponentially for the first values of n , saturates near ε level and then grows like $O(e^{cn})$.

Next we tune parameters as explained in Section 4. For $\Lambda = 5, 50$, in Fig. 5.2 (left) we plot the optimal values of θ against n . In Fig. 5.2 (right) we plot

$$\ln \max_{t \in [t_0, \Lambda t_0]} \|u(t) - \bar{u}_n(t)\|$$

(continuous line) and the logarithm of the corresponding values of the theoretical error estimate (dashed line) obtained in Theorem 2, versus n , once θ is optimal. We maintain $\alpha = 0.7$, $d = 0.6$ and $t_0 = 1$.

ILLUSTRATION 2. Take $\beta = 1.5$ and set

$$U(z) = \frac{z^{\beta-1}}{z^{\beta} + 1},$$

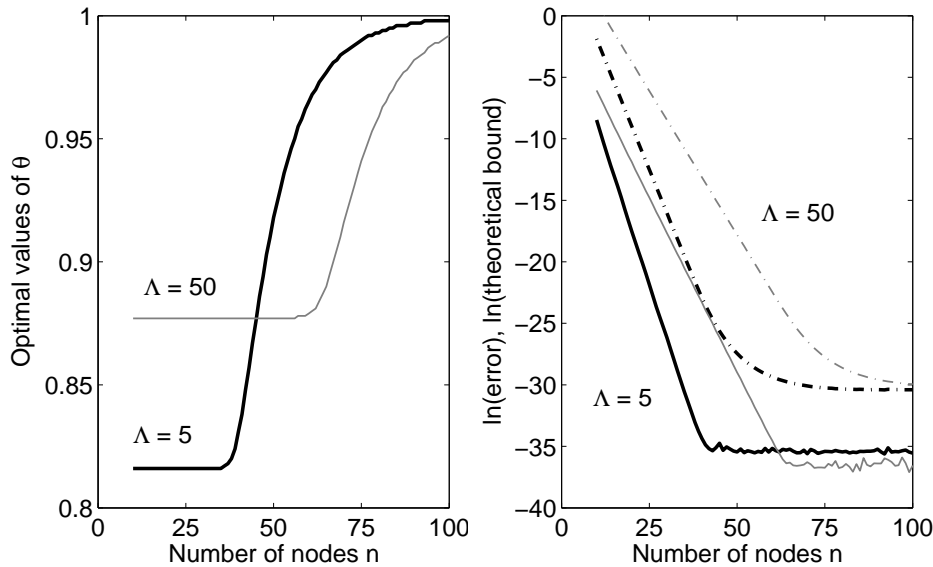


FIG. 5.2. Left: Optimal θ versus n . Right: Natural logarithms of $\max_{t \in [t_0, \Lambda t_0]} \|u(t) - \bar{u}_n(t)\|$ (continuous) and the theoretical estimate (dashed) versus n , for u in Illustration 1. The gray lines correspond to $\Lambda = 50$ and the black ones to $\Lambda = 5$.

i.e., $U(z)$ is the Laplace transform of

$$u(t) = M_\beta(-t^\beta),$$

where M_β stands for the Mittag-Leffler function of order β (see [18]). Notice that U satisfies (1.2) for any $\delta \in (\pi/3, \pi/2)$, with $\mu = 1$ and $M = 1/\sin(\beta(\pi - \delta))$. We consider here as exact solution the one computed with 500 nodes and take $\alpha = \pi/12$, $d = 0.25$ and $t_0 = 1$.

This example was already considered in [14]. In order to compare the performance of the strategy proposed in [14] with the one proposed in the present paper, we first compute $\bar{u}_n(t)$ by selecting the parameters as in [14]. In Fig. 5.3 (left) we plot in semilogarithmic scale the theoretical estimate and actual errors for $\Lambda = 2, 5$, which are acceptable. In Fig. 5.3 (right) we do the same for $\Lambda = 50$ and conclude that the approach in [14] is not at all useful for large values of Λ . However, the corresponding computation by using the strategy in Section 4, yields the plot in Fig. 5.4, which shows a satisfactory spectral order of convergence even for $\Lambda = 50$.

ILLUSTRATION 3. We consider the inhomogenous heat equation on the unit square $\Omega = (0, 1)^2$ with zero initial value and a convective heat flux at the boundary

$$\begin{cases} u_t(t, x) &= \Delta u(t, x) + f(x), \text{ for } x \in \Omega, t \geq 0, \\ \partial_\nu u(t, x) &= -u(t, x), \text{ for } x \in \partial\Omega, t \geq 0, \\ u(0, x) &= 0, \text{ for } x \in \Omega, \end{cases} \quad (5.1)$$

where f is the indicator function of the rectangle $R = [0.6, 0.8] \times [0.2, 0.8]$, i.e. $f = 1$ on R and $f = 0$ elsewhere.

Problem (5.1) is semidiscretized in space by using linear finite elements on a triangular grid. Denoting by $V_h \subset L^2(\Omega)$ the space of elements and by $U_h(z)$ the

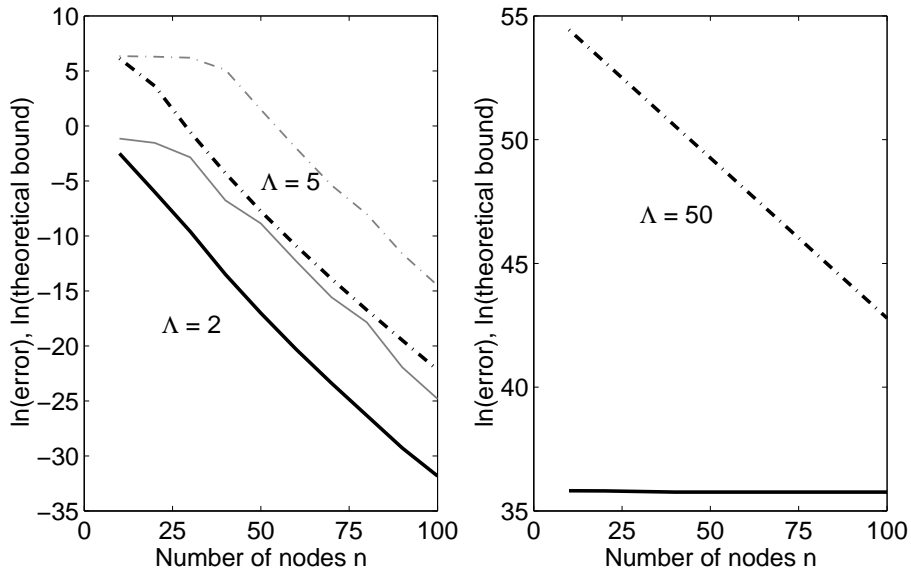


FIG. 5.3. Natural logarithms of $\max_{t \in [t_0, \Lambda t_0]} \|u(t) - \bar{u}_n(t)\|$ (continuous) and the theoretical estimate (dashed) versus n , for u in Illustration 2 proceeding as in [14] for $\delta = \pi/3$, $t_0 = 1$. The gray lines correspond to $\Lambda = 50$ and the black ones to $\Lambda = 5$.

Laplace transform of the semidiscrete solution $u_h(t)$, we get

$$U_h(z) = \frac{1}{z} (z - \Delta_h)^{-1} P_h f,$$

with $\Delta_h : V_h \rightarrow V_h$ the discrete laplacian and P_h the orthogonal projection of f onto V_h . Now, for fixed $h > 0$, we try to approximate $u_h(t)$ by inverting $U_h(z)$. Notice that, since Δ_h is definite negative, certainly $U_h(z)$ satisfies (1.2) for any $0 < \delta < \pi/2$ and $M = 1/(\mu_h \sin(\delta))$, with $-\mu_h$ the highest eigenvalue of Δ_h . Notice also that, working in coordinates relative to the standard basis of elements, $U_h(z)$ is represented by a vector valued mapping $\mathbf{U}_h(z)$ satisfying

$$zM_h \mathbf{U}_h(z) + S_h \mathbf{U}_h(z) = \frac{1}{z} \mathbf{f}_h,$$

where M_h and S_h stand for the mass and stiffness matrices and where \mathbf{f}_h is the vector formed by the scalar products of f with the elements of the basis. Thus, one evaluation of $U(z_k)$ at a given node z_k requires the solution of one linear system of the above form.

In the experiment we generate a mesh, shown in the left of Fig 5.5, with 542 triangles by means of the mesh generator Triangle [22]. Linear systems are solved using MATLABs sparse LU factorization UMFPACK. Since $u_h(t)$ is unknown, the errors are estimated in the $L^2(\Omega)$ -norm with respect to a reference solution $\bar{u}_{h,500}(t)$ obtained with 500 nodes. In the absence of precise information about ρ , both for this reference solution and for the rest of the approximations $\bar{u}_{h,n}(t)$ to $u_h(t)$, we tune $\theta = 1 - 1/n$, as indicated in Section 4. In Fig. 5.6, for the parameters $\alpha = 0.7$, $d = 0.6$, $t_0 = 0.01$ and $\theta = 1 - 1/n$, we plot $\ln \max_{t \in [t_0, \Lambda t_0]} \|\bar{u}_{h,500}(t) - \bar{u}_{h,n}(t)\|$ against n , for $\Lambda = 5, 50$. This plot shows the predicted behavior.

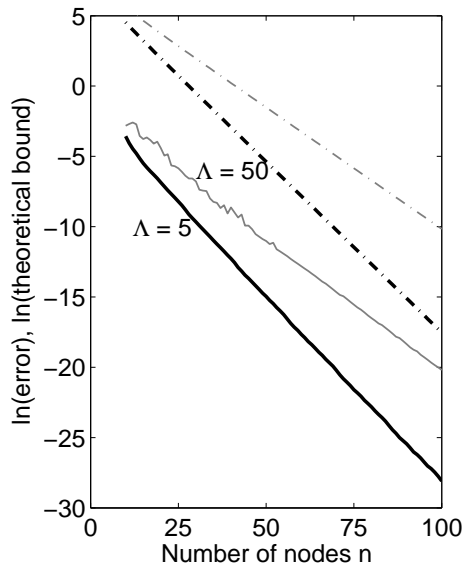


FIG. 5.4. Natural logarithm of $\max_{t \in [t_0, \Lambda t_0]} \|u(t) - \bar{u}_n(t)\|$ (continuous) and the theoretical estimate (dashed) versus n , for u in Illustration 2. The gray lines correspond to $\Lambda = 50$ and the black ones to $\Lambda = 5$.

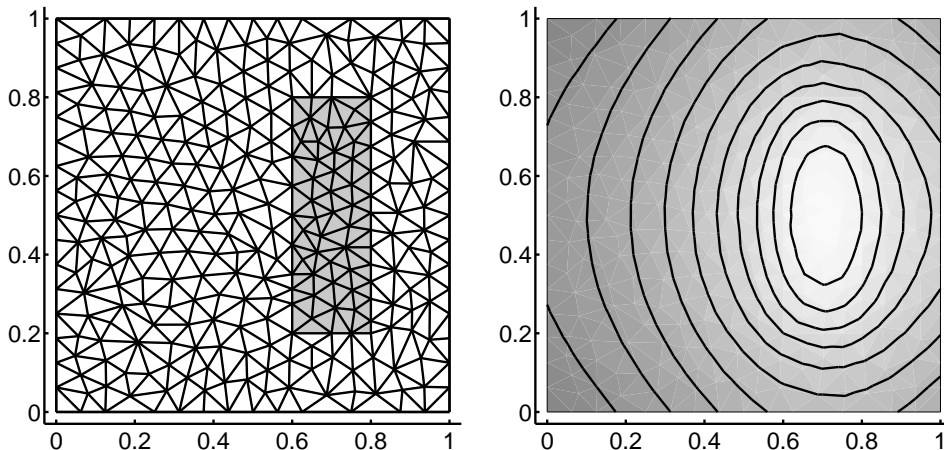


FIG. 5.5. Left: Mesh of Ω , with the set R indicated by darkgray. Right: Temperature distribution at $t = 0.5$ in false-color representation. (white corresponds to temperature 1 and black to 0)

ILLUSTRATION 4. We consider again the Laplace transform $U(z) = 1/(1+z)$ of the exponential function $u(t) = e^{-t}$ as in Illustration 1. The values of α , d and t_0 are again 0.7, 0.6 and 1, respectively.

We add on purpose perturbations of maximum size 10^{-4} to the evaluations of U at the required nodes. Thus, we use (3.1) with

$$U_k = U(z_k) + \eta_k, \quad -n \leq k \leq n,$$

with $|\eta_k| \leq \rho = 10^{-4}$. Now we try to approximate $u(t)$ without using the available information about ρ . In this situation, as explained in Section 4, we take $\theta = 1 - 1/n$.

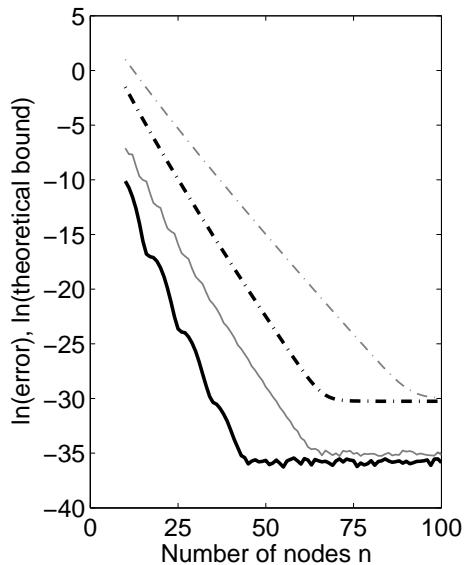


FIG. 5.6. Left: Natural logarithm of $\max_{t \in [t_0, \Lambda t_0]} \|u(t) - \bar{u}_n(t)\|$ (continuous) and the theoretical estimate (dashed) versus n , for u in Illustration 3. The gray lines correspond to $\Lambda = 5$ and the black ones to $\Lambda = 50$.

In fact, we compare two types of perturbations:

We first generate complex, random, independent perturbations η_k , in such a way that $|\eta_k|$ and $\arg(\eta_k)$ are uniformly distributed on $[0, 10^{-4}]$ and $[0, 2\pi]$, respectively. In Fig. 5.7 (left), we show the resulting actual error, which behaves much better than predicted by (4.2). The explanation is that cancellations are likely compensating the effects of the independent random perturbations. A finer analysis of the observed behavior is out of the scope of the present paper.

Secondly, for each $-n \leq k \leq n$, we consider the perturbation

$$\eta_k = 10^{-4} \exp(-i \arg(\omega_k(t_0))),$$

with $\omega_k(t_0)$ defined in (3.1). These perturbations correspond to the worst possible case in (3.2), for $t = t_0 = 1$. Now, the resulting actual error, plotted in Fig. 5.7 (right), fits quite well with (4.2).

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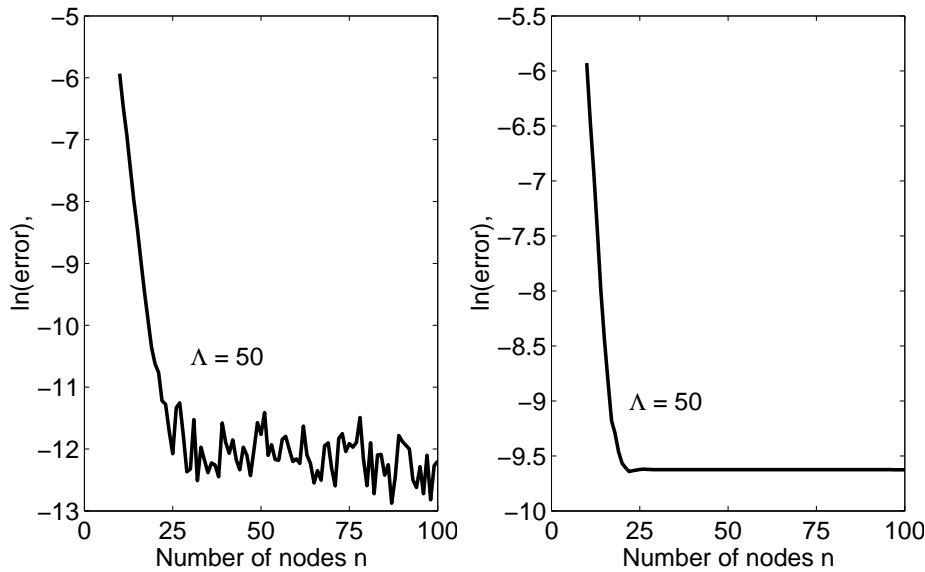


FIG. 5.7. $\ln \max_{t \in [t_0, \Lambda t_0]} (\|u(t) - \bar{u}_n(t)\|)$ versus n , for u in Illustration 4 with $\theta = 1 - 1/n$, $\alpha = 0.7$, $d = 0.6$, $t_0 = 1$ and $\Lambda = 50$. Left: Random perturbation. Right: Worst case perturbation.

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