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An approximation of matrix exponential by a truncated Laguerre series

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Abstract

The Laguerre functions $l^{\alpha}_{n,\tau}$, $n = 0, 1, \dots$, are constructed from generalized Laguerre polynomials. The functions $l^{\alpha}_{n,\tau}$ depend on two parameters: the scale $\tau > 0$ and the order of generalization $\alpha > -1$, and form an orthonormal basis in $L_2[0,\infty)$. Let the spectrum of a square matrix A lie in the open left half-plane. Then the matrix exponential $\mathcal{H}(t) = e^{At}$, $t > 0$, belongs to $L_2[0,\infty)$. Hence the matrix exponential $\mathcal{H}$ can be expanded in a series $\mathcal{H} = \sum_{n=0}^{\infty} S_{n,\tau,\alpha}\, l^{\alpha}_{n,\tau}$. An estimate of the norm $\left\| \mathcal{H} - \sum_{n=0}^{N} S_{n,\tau,\alpha}\, l^{\alpha}_{n,\tau} \right\|_{L_2[0,\infty)}$ is proposed. Finding the minimum of this estimate over τ and α is discussed. Numerical examples show that the optimal α is often almost 0, which essentially simplifies the problem.

1 Introduction

An approximate calculation of the matrix exponential $\mathcal{H}(t) = e^{At}$, $t > 0$, is of constant importance [10, 11, 13, 15, 20, 21] at least for solving linear differential equations

$$\dot{x}(t) = Ax(t) + f(t).$$

It is well-known that the solution of the equation satisfying the initial condition $x(0) = x_0$ can be expressed in terms of the matrix exponential:

$$x(t) = e^{At}x_0 + \int_0^t e^{A(t-s)} f(s)\, ds. \tag{*}$$

In a similar way, the nonlinear equation

$$\dot{x}(t) = Ax(t) + f\big(t, x(t)\big)$$

is often reduced to the Volterra integral equation

$$x(t) = e^{At}x_0 + \int_0^t e^{A(t-s)} f\big(s, x(s)\big)\, ds. \tag{**}$$

If we want to calculate solutions using these formulas (especially for many different free terms f), we need to know e^{At} for many values of t. Therefore, it is desirable to have a compact approximation of the matrix exponential $\mathcal{H}(t) = e^{At}$ in the form of a function depending on t.

We distinguish several variants of the problem of calculating the matrix exponential. First, one can calculate e^{A} or e^{At} for a finite number of t's. Second, one can try to obtain e^{At} in the form of a formula depending on the parameter t; the usual tools for this variant are the Jordan or Schur decompositions. Third, one can restrict himself to the calculation of $e^{At}b$ or $d^H e^{At} b$ (as a function of t or for discrete values of t), where b and d are column vectors (the knowledge of $e^{At}b$ or $d^H e^{At} b$ is enough for many applications). Fourth, one can try to construct an approximation for the matrix function $t \mapsto e^{At}$ that is simple and therefore convenient for further use.

We discuss the last problem. We deal with the problem of approximate representation of $\mathcal{H}(t) = e^{At}$, $t > 0$, in the form of a formula depending on the parameter t. The matrix A is assumed to be stable, i. e. the eigenvalues of A lie in the open left half-plane. We adhere two requirements: the approximation must be sufficiently accurate and the calculation of the approximation at any t can be performed quickly. Regarding the second requirement, we note that the exact representation of $\mathcal{H}$ (based on the

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Jordan decomposition) in the form of a formula may be very cumbersome if M is large, here $M\times M$ is the size of the matrix A (each of M^2 elements of the matrix function $\mathcal{H}$ is a linear combination of M functions of the form $t\mapsto t^j e^{\lambda_k t}$); therefore, it is inconvenient for large M.

We use the approximation

$$\mathcal{H}_{N,\tau,\alpha}(t)=\sum_{n=0}^{N} S_{n,\tau,\alpha}\, l^{\alpha}_{n,\tau}(t) \tag{***}$$

(depending on the parameters τ and α, see their discussion below), which is a linear combination of N (instead of M) scalar functions $l^{\alpha}_{n,\tau}$ with not very large N. Here $l^{\alpha}_{n,\tau}$ are known scalar functions, called the Laguerre functions, and $S_{n,\tau,\alpha}$ are constant matrices, which are rational function of the matrix A (maybe multiplied by one and the same matrix $(\tau\mathbf{1}-2A)^{-\alpha/2}$, where $\mathbf{1}$ is the identity matrix), see Propositions 4.1 and 4.2. Using the proposed approximation requires fewer arithmetic operations and is therefore more convenient than using exact $\mathcal{H}$. The calculation of the coefficients $S_{n,\tau,\alpha}$ is rather fast provided τ and α are given.

Sequence (***) converges to $\mathcal{H}$ for any τ and α, but the rate of convergence and hence the number N in (***) that provides high accuracy depends on τ and α. The aim of this paper is to estimate the accuracy of this approximation and use it for finding near-optimal τ and α. Numerical experiments show that for $N=10$ or $N=30$ such an approximation may be quite satisfactory.

Our method of estimating the accuracy requires the knowledge of the eigendecomposition $A=TDT^{-1}$ of A (we assume that it can be found by QR-algorithm). Of course, in such a case one can calculate e^{At} precisely by the formula $e^{At}=Te^{Dt}T^{-1}$. But we suppose that e^{At} can be used in further calculations like (*) or (**) for many different f's. Using the shorter formula (***) rather than $e^{At}=Te^{Dt}T^{-1}$ will save time.

Let us describe the contents of the paper more specifically. The *generalized Laguerre polynomials* are the functions

$$L^{\alpha}_n(t)=\frac{t^{-\alpha}e^t}{n!}\big(t^{n+\alpha}e^{-t}\big)^{(n)},\qquad \alpha>-1,\ t\ge 0,\ n=0,1,\dots.$$

We call *Laguerre functions* the modified Laguerre polynomials:

$$l^{\alpha}_{n,\tau}(t)=\sqrt{\frac{n!}{\Gamma(n+\alpha+1)}}\,\tau^{\frac{\alpha+1}{2}}\,t^{\frac{\alpha}{2}}\,e^{-\tau t/2}L^{\alpha}_n(\tau t),\qquad t\ge 0,\ \ n=0,1,\dots,$$

The Laguerre functions depend on two parameters: the order of generalization $\alpha>-1$ and the scale $\tau>0$. The most important and simple case is when $\alpha=0$.

It is known that $l^{\alpha}_{n,\tau}$ form an orthonormal basis in $L_2[0,\infty)$. Therefore the matrix exponential (impulse response)

$$\mathcal{H}(t)=e^{At},\qquad t>0,$$

can be expanded in the *Laguerre series*

$$\mathcal{H}=\sum_{n=0}^{\infty} S_{n,\tau,\alpha}\, l^{\alpha}_{n,\tau}$$

with matrix coefficients $S_{n,\tau,\alpha}$. The coefficient $S_{n,\tau,\alpha}$ can be interpreted (Proposition 4.2) as the result of the substitution of A in the function $\lambda\mapsto s_{n,\tau,\alpha,\lambda}$, where

$$s_{n,\tau,\alpha,\lambda}=\int_0^{\infty} e^{\lambda t}\, l^{\alpha}_{n,\tau}(t)\,dt.$$

Since the matrix exponential $\mathcal{H}$ is a linear combination of functions of the form $t\mapsto t^j e^{\lambda_k t}$ (where λ_k are eigenvalues of A), which resemble $l^{\alpha}_{n,\tau}$, it is natural to expect that the Laguerre series converges rather fast and hence its truncation or partial sum

$$\mathcal{H}_{N,\tau,\alpha}=\sum_{n=0}^{N} S_{n,\tau,\alpha}\, l^{\alpha}_{n,\tau}$$

approximates $\mathcal{H}$ quite well.

The task of this paper is estimating the accuracy $\|\mathcal{H}-\mathcal{H}_{N,\tau,\alpha}\|_{L_2}$ and choosing τ and α that provide the best estimate. The idea of the paper is as follows. We describe (Theorem 5.2) the estimate of $\|\mathcal{H}-\mathcal{H}_{N,\tau,\alpha}\|_{L_2}$ in terms of the quantities

$$\varphi(N,\tau,\alpha)=\sum_{k=1}^{M}\zeta(N,\tau,\alpha,\lambda_k),$$
$$\psi(N,\tau,\alpha)=\max_k \zeta(N,\tau,\alpha,\lambda_k),$$

where λ_k, $k=1,2\dots,M$, are eigenvalues of A, and

$$\zeta(N,\tau,\alpha,\lambda)=\int_0^{\infty}\Big|e^{\lambda t}-\sum_{n=0}^{N} s_{n,\tau,\alpha,\lambda}\, l^{\alpha}_{n,\tau}(t)\Big|^2\,dt.$$

We recommend to choose τ and α so that $\varphi(N,\tau,\alpha)$ be minimal (alternatively, $\psi(N,\tau,\alpha)$ could be minimised). Numerical experiments show that the optimal α is often close to 0. Optimization with respect to τ reduces N in (***), which speeds up further calculations.

The most popular algorithm of calculating e^A is the scaling and squaring method, see, e. g., [2, 8, 14, 19, 27, 30]. But this approach is not suitable for our aims, because we would like to have e^{At} in the form of a function depending on t.

There are many papers devoted to the approximation of impulse responses and matrix exponential by the truncated Laguerre series and the optimal choice of τ and α, see, e. g., [3, 4, 5, 22, 24, 26, 28, 29, 33] and references therein. It is natural to compare the present paper with them. In papers [3, 5, 24, 26, 33] the problem of approximation of a scalar impulse response (in our notation it corresponds to the function $t\mapsto d^He^{At}b$) by a truncated Laguerre series is considered; we use in Proposition 6.1 the main idea of these papers.

Paper [29] discusses the approximation of the vector function $t\mapsto e^{At}b$ using the Laguerre polynomials, but it uses the different expansion

$$e^{At}\approx\sum_{n=0}^{N}s_{n,\tau,\alpha,t}\,l^{\alpha}_{n,\tau}(A)$$

(here the coefficients $s_{n,\tau,\alpha,t}$ are scalar, while in formula (5) below the similar coefficients $S_{n,\tau,\alpha}$ are matrix); the convenience of this approach is that $l^{\alpha}_{n,\tau}(A)$ can be calculated recursively.

The topic of paper [22] is closest to the present one. It is devoted to the approximation of the matrix exponential $t\mapsto e^{At}$ by the truncated Laguerre series. In [22] only ordinary Laguerre functions (i. e. with $\alpha=0$) are considered. The optimization over τ is also discussed, but in different notation (as a preliminary scaling of A): the goal consists in minimization of $\big\|(2A+\tau\mathbf{1})(2A-\tau\mathbf{1})^{-1}\big\|$, which leads to fast asymptotic decay of $S_{n,\tau,0}$, see Corollary 7.2.

In [28] the matrix exponential $t\mapsto e^{At}$ is approximated by the truncated Laguerre series depending on both τ and α; the parameters τ and α, which give the fastest convergence, are found from numerical experiments; the results obtained show that the optimal value of α can be greater than 10.

The paper is organized as follows. Sections 2 and 3 are devoted to definitions and notation. In Section 4, we derive some formulas for Laguerre coefficients. In Section 5, we describe the main estimate. In Section 6, we recall [3, 4, 5] formulas for calculating the derivative of ζ with respect to τ. They simplify the search for the minimum with respect to τ only. The problem of finding minimum over τ only arises, for example, when we restrict ourselves to the case $\alpha=0$; some simplified formulas for the case $\alpha=0$ are collected in Section 7. In Section 8, we present the recommended algorithm of finding the optimal τ and α. In Section 9, we describe the results of some numerical experiments.

We use 'Wolfram Mathematica' [36] for our computer calculations.

2 The definition of Laguerre functions

In this section, we recall some definitions.

The functions

$$L^{\alpha}_n(t)=\frac{t^{-\alpha}e^t}{n!}\big(t^{n+\alpha}e^{-t}\big)^{(n)}=\sum_{k=0}^{n}(-1)^k\binom{n+\alpha}{n-k}\frac{t^k}{k!},\qquad t\ge0,\ \alpha>-1,\ n=0,1,\dots.$$

are called [1, p. 775], [9, p. 31], [16, p. 71] *generalized Laguerre polynomials*. The special cases

$$L_n(t)=\frac{e^t}{n!}\big(t^ne^{-t}\big)^{(n)},\qquad t\ge0,\ n=0,1,\dots.$$

of these functions are called (*ordinary*) *Laguerre polynomials*. Actually, L^{α}_n is a polynomial of degree n. It is well-known [32, Theorem 5.7.1], [18, p. 88], [23, § 8] that the functions L^{α}_n form an orthogonal basis in $L_2[0,\infty)$ with the weight function $t\mapsto t^{\alpha}e^{-t}$:

$$\int_0^{\infty}t^{\alpha}e^{-t}L^{\alpha}_n(t)\,L^{\alpha}_m(t)\,dt=\frac{\Gamma(n+\alpha+1)}{n!}\,\delta_{nm},\qquad n,m=0,1,\dots,$$

where δ_{nm} is the Kronecker symbol. We note that the ordinary polynomials L_n are normalized, but the generalized ones L^{α}_n, $\alpha\ne0$, are not.

Let $\tau>0$ be a given number. It plays a role of a time scale. We call the family of functions

$$\begin{aligned}l^{\alpha}_{n,\tau}(t)&=\sqrt{\frac{n!}{\Gamma(n+\alpha+1)}}\,\tau^{\frac{\alpha+1}{2}}\,t^{\frac{\alpha}{2}}\,e^{-\tau t/2}L^{\alpha}_n(\tau t)\\&=\sqrt{\frac{\tau n!}{\Gamma(n+\alpha+1)}}\,e^{-\tau t/2}\sum_{k=0}^{n}(-1)^k\binom{n+\alpha}{n-k}\frac{(\tau t)^{k+\alpha/2}}{k!},\qquad n=0,1,\dots.\end{aligned}\tag{1}$$

the (*generalized*) *Laguerre functions*. In particular,

$$l_{n,\tau}(t) = l^0_{n,\tau}(t) = \sqrt{\tau}\, e^{-\tau t/2} L_n(\tau t), \qquad t \ge 0, \; n = 0, 1, \dots.$$

Evidently, the Laguerre functions $l^\alpha_{n,\tau}$ form an orthonormal basis in $L_2[0,\infty)$ (without weight):

$$\int_0^\infty l^\alpha_{n,\tau}(t)\, l^\alpha_{m,\tau}(t)\, dt = \delta_{nm}, \qquad t \ge 0, \; n, m = 0, 1, \dots.$$

3 Laguerre series for $\mathcal{H}$

In this section, we introduce some notation.

Let M be a positive integer. We denote by $\mathbb{C}^{M\times M}$ the linear space of all matrices of the size $M \times M$; the symbol $\mathbf{1} \in \mathbb{C}^{M\times M}$ denotes the identity matrix.

For a matrix $C = \{C_{ij}\} \in \mathbb{C}^{M\times M}$, we denote by $\|C\|_{2\to 2}$ the norm induced by the Euclidean norm $\|\cdot\|_2$ on $\mathbb{C}^M$ and by

$$\|C\|_F = \sqrt{\sum_{i=1}^M \sum_{j=1}^M |C_{ij}|^2}$$

the Frobenius norm [11, p. 71]. It is easy to show that

$$\begin{aligned} \|A\|_{2\to 2} &\le \|A\|_F, \\ \|AB\|_F &\le \|A\|_{2\to 2} \cdot \|B\|_F, \\ \|AB\|_F &\le \|A\|_F \cdot \|B\|_{2\to 2}, \\ \|Ax\|_2 &\le \|A\|_F \cdot \|x\|_2. \end{aligned}$$

By default, we use for matrices $C \in \mathbb{C}^{M\times M}$ the Frobenius norm. We denote by $\sigma(C)$ the spectrum (the set of all eigenvalues) of a square matrix C.

Let $A \in \mathbb{C}^{M\times M}$ be a given matrix and $U \subseteq \mathbb{C}$ be an open set that contains the spectrum $\sigma(A)$ of the matrix A, and let $f : U \to \mathbb{C}$ be a holomorphic function. The matrix $f(A)$ is defined [13, 25] by the formula

$$f(A) = \frac{1}{2\pi i} \int_\Gamma f(\lambda)(\lambda \mathbf{1} - A)^{-1}\, d\lambda,$$

where Γ is contained in U and surrounds $\sigma(A)$. The most important example of a function f for applications is the function $\lambda \mapsto e^{\lambda t}$. The result of its action on A is denoted by the symbol e^{At}. It is well-known that the matrix exponential possesses the following properties:

$$e^{A(t+s)} = e^{At} e^{As}, \qquad \left(e^{At}\right)' = A e^{At}, \qquad e^{A\cdot 0} = \mathbf{1}.$$

We recall that eigenvalues and eigenvectors of A can be calculated [36] with high backward stability by the QR-algorithm [11, 13, 35].

Proposition 3.1 ([6, p. 27])**.** *Let*

$$\beta = \max\{\operatorname{Re}\lambda : \lambda \in \sigma(A)\}.$$

Then for any $\gamma > \beta$ there exists K such that

$$\|e^{At}\| \le K\, e^{\gamma t}, \qquad t \ge 0.$$

We recall [7, ch. VII, § 1, Theorem 5], [17, ch. 1, § 5] that for any square matrix A,

$$f(A) = \sum_{k=1}^m \sum_{j=0}^{w_k - 1} \frac{d^j f}{d\lambda^j}(\lambda_k) \frac{N_k^j}{j!}, \tag{2}$$

where λ_k are eigenvalues of A, m is a number of distinct eigenvalues λ_k, w_k are their multiplicities, and N_k are spectral nilpotents; in particular, $N_k^0 = P_k$ are spectral projectors. If all eigenvalues are simple, then

$$f(A) = \sum_{k=1}^M f(\lambda_k) P_k.$$

For the exponential function $\lambda \mapsto e^{\lambda t}$ formula (2) takes the form

$$e^{At} = \sum_{k=1}^m \sum_{j=0}^{w_k - 1} t^j e^{\lambda_k t} \frac{N_k^j}{j!}. \tag{3}$$

In particular, if all eigenvalues are simple, then

$$e^{At} = \sum_{k=1}^{M} e^{\lambda_k t} P_k.$$

Let $A \in \mathbb{C}^{M\times M}$ be a given matrix. We assume that A is *stable*, i. e. the eigenvalues of A lie in the open left half-plane. We discuss the expansion of the function

$$\mathcal{H}(t) = e^{At}, \qquad t > 0,$$

in the series of Laguerre functions. We call $\mathcal{H}$ the *matrix exponential of* A or the *impulse response of the differential equation*

$$\dot{x}(t) = Ax(t) + f(t).$$

We recall that the generalized Laguerre functions (1) form an orthonormal basis in $L_2[0,\infty)$; here the scale parameter $\tau > 0$ and the order of generalization $\alpha > -1$ can be taken arbitrarily. Therefore the matrix exponential $\mathcal{H}$ can be represented in the form of the *Laguerre series*

$$\mathcal{H} = \sum_{n=0}^{\infty} S_{n,\tau,\alpha}\, l_{n,\tau}^{\alpha},$$

where the Laguerre coefficients

$$S_{n,\tau,\alpha} = \int_0^{\infty} \mathcal{H}(t)\, l_{n,\tau}^{\alpha}(t)\, dt \tag{4}$$

are matrices. Since the matrix exponential $\mathcal{H}$ is a linear combination of functions of the form $t \mapsto t^j e^{\lambda_k t}$, it is natural to expect that the series converges quite quickly and hence its N-truncation

$$\mathcal{H}_{N,\tau,\alpha}(t) = \sum_{n=0}^{N} S_{n,\tau,\alpha}\, l_{n,\tau}^{\alpha}(t) \tag{5}$$

with relatively small N approximates $\mathcal{H}$ well enough.

The aim of this paper is to estimate the quantity

$$\|\mathcal{H} - \mathcal{H}_{N,\tau,\alpha}\|_{L_2[0,\infty)} = \sqrt{\int_0^{\infty} \big\|\mathcal{H}(t) - \mathcal{H}_{N,\tau,\alpha}(t)\big\|_F^2\, dt},$$

where $\|\cdot\|_F$ is the Frobenius norm, and to give recommendations on the optimal choice of τ and α based on it.

4 The Laguerre coefficients of h_λ

In the simplest case, when the matrix A has the size 1×1, the problem of construction of approximation (5) is reduced to the calculation of Laguerre coefficients $s_{n,\tau,\alpha,\lambda}$ of the function $t \mapsto e^{\lambda t}$; we do it in Proposition 4.1. Then we describe the expression of $S_{n,\tau,\alpha}$ in terms of $s_{n,\tau,\alpha,\lambda}$ (Proposition 4.2).

For $\operatorname{Re}\lambda < 0$ (here and below Re means the real part of a complex number), we consider the auxiliary function

$$h_\lambda(t) = e^{\lambda t}, \qquad t > 0.$$

It is straightforward to verify that

$$\|h_\lambda\|_{L_2[0,\infty)} = \frac{1}{\sqrt{-2\operatorname{Re}\lambda}}.$$

Our interest in the function h_λ is explained by the following. If λ is an eigenvalue of A (recall that $\operatorname{Re}\lambda < 0$) and v is the corresponding normalized eigenvector, then the function

$$x_\lambda(t) = \mathcal{H}(t)v$$

can be represented as

$$x_\lambda(t) = h_\lambda(t)v.$$

Let us first perform some calculations with the functions h_λ. They can be interpreted as the approximation of the matrix exponential $\mathcal{H}$ by the truncated Laguerre series (5) when A is a matrix of the size 1×1 whose only element equals λ.

We denote by $s_{n,\tau,\alpha,\lambda}$ the Laguerre coefficients of the function h_λ in the orthonormal basis $l_{n,\tau}^{\alpha}$:

$$s_{n,\tau,\alpha,\lambda} = \int_0^{\infty} h_\lambda(t)\, l_{n,\tau}^{\alpha}(t)\, dt, \qquad \operatorname{Re}\lambda < 0. \tag{6}$$

Clearly, $s_{n,\tau,\alpha,\lambda}$ are real for real λ. Therefore, from the Schwartz reflection principle for holomorphic functions [12, theorem 7.5.2], it follows that

$$\overline{s_{n,\tau,\alpha,\lambda}} = s_{n,\tau,\alpha,\bar{\lambda}}, \tag{7}$$

where the bar means the complex conjugate. Representation (7) is useful for symbolic calculation of derivatives.

Proposition 4.1. *Let* $\operatorname{Re}\lambda < 0$. *Then*

$$s_{n,\tau,\alpha,\lambda} = \frac{\Gamma(\alpha/2+1)}{(\tau/2-\lambda)^{\alpha/2+1}}\,\tau^{\frac{\alpha+1}{2}}\binom{n+\alpha}{n}\sqrt{\frac{n!}{\Gamma(n+\alpha+1)}}\;{}_2F_1\big(-n,\alpha/2+1,\alpha+1,\tau/(\tau/2-\lambda)\big), \tag{8}$$

where ${}_2F_1$ *is the hypergeometric function. In particular,*

$$s_{n,\tau,0,\lambda} = -\frac{2\sqrt{\tau}(2\lambda+\tau)^n}{(2\lambda-\tau)^{n+1}}, \qquad n = 0,1,\dots.$$

Remark 1. We note that the function $z \mapsto {}_2F_1\big(-n,\alpha/2+1,\alpha+1,z\big)$ is a polynomial of degree n, since [16, p. 10] its first argument $-n$ is a negative integer. Thus it is calculated quickly and accurately.

Proof. We begin with the formula [31, formula (16)]

$$\int_0^\infty t^\beta e^{-\sigma t} L_n^\alpha(\tau t) L_k^\beta(\sigma t)\,dt = \binom{n+\alpha}{n-k}\binom{k+\beta}{k}\frac{\tau^k\,\Gamma(\beta+1)}{\sigma^{\beta+k+1}}\;{}_2F_1\big(-n+k,\beta+k+1,\alpha+k+1,\tau/\sigma\big).$$

We have (see (1) and note that $L_0^\beta(t) = 1$ for all $t \ge 0$ and $\binom{\alpha/2}{0} = 1$)

$$\begin{aligned} s_{n,\tau,\alpha,\lambda} &= \int_0^\infty e^{\lambda t}\sqrt{\frac{n!}{\Gamma(n+\alpha+1)}}\,\tau^{\frac{\alpha+1}{2}}\,t^{\frac{\alpha}{2}}\,e^{-\tau t/2}L_n^\alpha(\tau t)\,dt \\ &= \sqrt{\frac{n!}{\Gamma(n+\alpha+1)}}\,\tau^{\frac{\alpha+1}{2}}\int_0^\infty e^{(\lambda-\tau/2)t}\,t^{\frac{\alpha}{2}}\,L_n^\alpha(\tau t)\,dt \\ &= \sqrt{\frac{n!}{\Gamma(n+\alpha+1)}}\,\tau^{\frac{\alpha+1}{2}}\int_0^\infty t^{\frac{\alpha}{2}}\,e^{(\lambda-\tau/2)t}\,L_n^\alpha(\tau t)\,L_0^{\alpha/2}\big((\tau/2-\lambda)t\big)\,dt \\ &= \sqrt{\frac{n!}{\Gamma(n+\alpha+1)}}\,\tau^{\frac{\alpha+1}{2}}\binom{n+\alpha}{n}\frac{\Gamma(\alpha/2+1)}{(\tau/2-\lambda)^{\alpha/2+1}} \\ &\quad\times {}_2F_1\big(-n,\alpha/2+1,\alpha+1,\tau/(\tau/2-\lambda)\big). \qquad \square \end{aligned}$$

Remark 2. In a similar way one can derive the formula for the Laguerre coefficients of the functions $t \mapsto t^j e^{\lambda t}$ which correspond to generalized eigenvectors of A:

$$q_{n,\tau,\alpha,\lambda} = \int_0^\infty t^j e^{\lambda t}\, l_{n,\tau}^\alpha(t)\,dt = \sqrt{\frac{n!}{\Gamma(n+\alpha+1)}}\,\tau^{\frac{\alpha+1}{2}}\binom{n+\alpha}{n}\frac{\Gamma(\alpha/2+j+1)}{(\tau/2-\lambda)^{\alpha/2+1}}\;{}_2F_1\big(-n,\alpha/2+j+1,\alpha+1,\tau/(\tau/2-\lambda)\big).$$

Proposition 4.2. *Let the spectrum of* A *lie in the open left half-plane. Then the coefficient* $S_{n,\tau,\alpha}$ *is the function* $\lambda \mapsto s_{n,\tau,\alpha,\lambda}$ *of* A.

Proof. Let n be a non-negative integer, $\tau > 0$, and $\alpha > -1$ be fixed. For brevity, we set $f(\lambda) = s_{n,\tau,\alpha,\lambda}$. From Proposition 4.1 it is seen that f is holomorphic in the open left half-plane $\operatorname{Re}\lambda < 0$. We recall that

$$s_{n,\tau,\alpha,\lambda} = \int_0^\infty h_\lambda(t)\, l_{n,\tau}^\alpha(t)\,dt = \int_0^\infty e^{\lambda t}\, l_{n,\tau}^\alpha(t)\,dt.$$

From this formula, it is clear that

$$\frac{\partial s_{n,\tau,\alpha,\lambda}}{\partial\lambda} = \int_0^\infty t\,e^{\lambda t}\, l_{n,\tau}^\alpha(t)\,dt, \qquad \frac{\partial^j s_{n,\tau,\alpha,\lambda}}{\partial\lambda^j} = \int_0^\infty t^j\,e^{\lambda t}\, l_{n,\tau}^\alpha(t)\,dt.$$

From (3) and (4), it follows that

$$\begin{aligned} S_{n,\tau,\alpha} &= \int_0^\infty e^{At}\, l_{n,\tau}^\alpha(t)\,dt \\ &= \int_0^\infty \sum_{k=1}^m \sum_{j=0}^{w_k-1} t^j e^{\lambda_k t}\frac{N_k^j}{j!}\, l_{n,\tau}^\alpha(t)\,dt \\ &= \sum_{k=1}^m \sum_{j=0}^{w_k-1} \frac{N_k^j}{j!}\int_0^\infty t^j e^{\lambda_k t}\, l_{n,\tau}^\alpha(t)\,dt \\ &= \sum_{k=1}^m \sum_{j=0}^{w_k-1} \frac{N_k^j}{j!}\frac{\partial^j s_{n,\tau,\alpha,\lambda_k}}{\partial\lambda^j}, \end{aligned}$$

which, by (2), equals the function $\lambda \mapsto s_{n,\tau,\alpha,\lambda}$ of A. $\square$

Let τ and α be given. Then Propositions 4.1 and 4.2 (see also Corollary 7.2 below) propose the way to calculate the coefficients $S_{n,\tau,\alpha}$:

$$S_{n,\tau,\alpha} = \Gamma(\alpha/2+1)(\tau\mathbf{1}/2-A)^{-\alpha/2-1}\,\tau^{\frac{\alpha+1}{2}}\binom{n+\alpha}{n}\sqrt{\frac{n!}{\Gamma(n+\alpha+1)}}\;{}_2F_1\big(-n,\alpha/2+1,\alpha+1,\tau(\tau\mathbf{1}/2-A)^{-1}\big).$$

We do not discuss this calculation in detail in this paper. We only note that by Remark 1 ${}_2F_1\big(-n,\alpha/2+1,\alpha+1,\tau(\tau\mathbf{1}/2-A)^{-1}\big)$ is a special polynomial in $\tau(\tau\mathbf{1}/2-A)^{-1}$ of degree n; therefore, it would be convenient to calculate powers of $\tau(\tau\mathbf{1}/2-A)^{-1}$ a priori. The other matrix that should be calculated in advance is the power $(\tau\mathbf{1}/2-A)^{-\alpha/2-1}$. Having found $S_{n,\tau,\alpha}$, we obtain the approximation

$$\mathcal{H}(t)\approx\sum_{n=0}^{N}S_{n,\tau,\alpha}\,l^{\alpha}_{n,\tau}(t).$$

5 The estimate of accuracy

In this section, we assume that $\alpha>-1$ and $\tau>0$ are given.

In order for the truncated Laguerre series (5) approximate the matrix exponential $\mathcal{H}$ well enough, first of all, the truncated Laguerre series

$$h_{N,\tau,\alpha,\lambda}=\sum_{n=0}^{N}s_{n,\tau,\alpha,\lambda}\,l^{\alpha}_{n,\tau}$$

should approximate the function h_λ for all $\lambda\in\sigma(A)$. In this section, we discuss the inverse problem: how to estimate $\big\|\mathcal{H}-\mathcal{H}_{N,\tau,\alpha}\big\|_{L_2}$ in terms of $\big\|h_{\lambda_k}-h_{N,\tau,\alpha,\lambda_k}\big\|_{L_2}$, where λ_k runs over the eigenvalues of A.

For $\operatorname{Re}\lambda<0$ and a natural number N, we denote by $\zeta(N,\tau,\alpha,\lambda)$ the square of the accuracy of the approximation of the function h_λ by its N-truncated Laguerre series:

$$\zeta(N,\tau,\alpha,\lambda)=\int_0^\infty\Big|e^{\lambda t}-\sum_{n=0}^{N}s_{n,\tau,\alpha,\lambda}\,l^{\alpha}_{n,\tau}(t)\Big|^2\,dt. \tag{9}$$

Clearly, we can rewrite this formula as

$$\begin{aligned}\zeta(N,\tau,\alpha,\lambda)&=\Big\|h_\lambda-\sum_{n=0}^{N}s_{n,\tau,\alpha,\lambda}\,l^{\alpha}_{n,\tau}\Big\|^2_{L_2}\\&=\Big\|\sum_{n=N+1}^{\infty}s_{n,\tau,\alpha,\lambda}\,l_{n,\tau}\Big\|^2_{L_2}\\&=\sum_{n=N+1}^{\infty}|s_{n,\tau,\alpha,\lambda}|^2.\end{aligned}\tag{10}$$

Proposition 5.1. *Let $A\in\mathbb{C}^{M\times M}$ be a diagonal matrix with diagonal elements λ_k, $\operatorname{Re}\lambda_k<0$, $k=1,2,\dots,M$. Then for the number*

$$\|\mathcal{H}-\mathcal{H}_{N,\tau,\alpha}\|_{L_2}=\sqrt{\int_0^\infty\big\|\mathcal{H}(t)-\mathcal{H}_{N,\tau,\alpha}(t)\big\|_F^2\,dt},$$

where $\|\cdot\|_F$ is the Frobenius norm on $\mathbb{C}^{n\times n}$, we have

$$\|\mathcal{H}-\mathcal{H}_{N,\tau,\alpha}\|_{L_2}=\sqrt{\sum_{k=1}^{M}\zeta(N,\tau,\alpha,\lambda_k)}\le\sqrt{M\max_k\zeta(N,\tau,\alpha,\lambda_k)},$$

where λ_k are the eigenvalues of A and the function ζ is defined by (9).

Proof. By assumption, the matrix A has the form

$$A=\begin{pmatrix}\lambda_1&0&\dots&0\\0&\lambda_2&\dots&0\\\vdots&\vdots&\ddots&\vdots\\0&0&\dots&\lambda_M\end{pmatrix}.$$

Therefore,

$$\mathcal{H}(t)=\begin{pmatrix}h_{\lambda_1}(t)&0&\dots&0\\0&h_{\lambda_2}(t)&\dots&0\\\vdots&\vdots&\ddots&\vdots\\0&0&\dots&h_{\lambda_M}(t)\end{pmatrix}$$

and

$$\mathcal{H}_{N,\tau,\alpha}(t)=\begin{pmatrix}\sum_{n=0}^{N}s_{n,\tau,\alpha,\lambda_1}\,l^{\alpha}_{n,\tau}(t) & 0 & \dots & 0\\ 0 & \sum_{n=0}^{N}s_{n,\tau,\alpha,\lambda_2}\,l^{\alpha}_{n,\tau}(t) & \dots & 0\\ \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & \dots & \sum_{n=0}^{N}s_{n,\tau,\alpha,\lambda_M}\,l^{\alpha}_{n,\tau}(t)\end{pmatrix}.$$

Hence, by the definition of the Frobenius norm,

$$\left\|\mathcal{H}(t)-\mathcal{H}_{N,\tau,\alpha}(t)\right\|_F^2=\sum_{k=1}^{M}\left|h_{\lambda_k}(t)-\sum_{n=0}^{N}s_{n,\tau,\alpha,\lambda_k}\,l^{\alpha}_{n,\tau}(t)\right|^2.$$

Consequently, (recall that $\operatorname{Re}\lambda_k<0$)

$$\begin{aligned}\sqrt{\int_0^{\infty}\left\|\mathcal{H}(t)-\mathcal{H}_{N,\tau,\alpha}(t)\right\|_F^2\,dt}&=\sqrt{\int_0^{\infty}\sum_{k=1}^{M}\left|h_{\lambda_k}(t)-\sum_{n=0}^{N}s_{n,\tau,\alpha,\lambda_k}\,l^{\alpha}_{n,\tau}(t)\right|^2dt}\\&=\sqrt{\sum_{k=1}^{M}\int_0^{\infty}\left|h_{\lambda_k}(t)-\sum_{n=0}^{N}s_{n,\tau,\alpha,\lambda_k}\,l^{\alpha}_{n,\tau}(t)\right|^2dt}\\&=\sqrt{\sum_{k=1}^{M}\zeta(N,\tau,\alpha,\lambda_k)}.\quad\square\end{aligned}$$

Now let us suppose that the matrix A is *diagonalizable*; this means that there exists an invertible matrix T and a diagonal matrix D such that

$$A=TDT^{-1}.$$

In such a case, the diagonal elements of D are the eigenvalues of A and the columns of T are the corresponding eigenvectors. Without loss of generality we can assume that the columns of T have unit Euclidian norm. The matrix D can be interpreted as the Jordan form of the matrix A; thus, a diagonalizable matrix has (complex) Jordan blocks of the size 1×1 only. It is clear that for a diagonalizable matrix A,

$$\begin{aligned}\mathcal{H}(t)&=e^{At}=Te^{Dt}T^{-1}, && t>0,\\ \mathcal{H}_{N,\tau,\alpha}(t)&=\sum_{n=0}^{N}TS_{n,\tau,\alpha,D}T^{-1}\,l^{\alpha}_{n,\tau}(t), && t>0.\end{aligned}$$

Here $S_{n,\tau,\alpha,D}$ are matrices (4) constructed by the matrix exponential $\mathcal{H}_D(t)=e^{Dt}$ of D, but not by the matrix exponential $\mathcal{H}(t)=e^{At}$ of A.

Recall that we use the Frobenius norm in the space $\mathbb{C}^{M\times M}$.

Theorem 5.2. *Let $A\in\mathbb{C}^{M\times M}$ and λ_k, $k=1,2,\dots,M$, be eigenvalues of A. Then*

$$\sqrt{\max_k\zeta(N,\tau,\alpha,\lambda_k)}\le\|\mathcal{H}-\mathcal{H}_{N,\tau,\alpha}\|_{L_2[0,\infty)}\tag{11}$$

and (*provided that A is diagonalizable*)

$$\|\mathcal{H}-\mathcal{H}_{N,\tau,\alpha}\|_{L_2[0,\infty)}\le\varkappa(T)\sqrt{\sum_{k=1}^{M}\zeta(N,\tau,\alpha,\lambda_k)}\le\varkappa(T)\sqrt{M\max_k\zeta(N,\tau,\alpha,\lambda_k)},\tag{12}$$

where $\varkappa(T)=\|T\|_{2\to2}\cdot\|T^{-1}\|_{2\to2}$ is the condition number [13, p. 63] of T.

Proof. Let λ be an eigenvalue of A and v be the corresponding normalized eigenvector. Since $\mathcal{H}(t)$ and $S_{n,\tau,\alpha,\lambda}$ are respectively the functions $\lambda\mapsto h_\lambda(t)$ and $\lambda\mapsto s_{n,\tau,\alpha,\lambda}$ of A (Proposition 4.2), v is also the eigenvector of $\mathcal{H}(t)$ and $S_{n,\tau,\alpha}$, and it corresponds to the eigenvalues $h_\lambda(t)$ and $s_{n,\tau,\alpha,\lambda}$:

$$\begin{aligned}\mathcal{H}(t)v&=h_\lambda(t)v,\\ \mathcal{H}_{N,\tau,\alpha}(t)v&=\Big(\sum_{n=0}^{N}S_{n,\tau,\alpha}\,l^{\alpha}_{n,\tau}(t)\Big)v=\Big(\sum_{n=0}^{N}s_{n,\tau,\alpha,\lambda}\,l^{\alpha}_{n,\tau}(t)\Big)v.\end{aligned}$$

Therefore,

$$\begin{aligned}
\big\|\mathcal{H}-\mathcal{H}_{N,\tau,\alpha}\big\|_{L_2} &\geq \big\|(\mathcal{H}-\mathcal{H}_{N,\tau,\alpha})v\big\|_{L_2}\\
&= \sqrt{\int_0^\infty \big\|\big(\mathcal{H}(t)-\mathcal{H}_{N,\tau,\alpha}(t)\big)v\big\|^2\,dt}\\
&= \sqrt{\int_0^\infty \Big\|\Big(h_\lambda(t)-\sum_{n=0}^N s_{n,\tau,\alpha,\lambda}\, l_{n,\tau}^\alpha(t)\Big)v\Big\|^2\,dt}\\
&= \sqrt{\int_0^\infty \Big|h_\lambda(t)-\sum_{n=0}^N s_{n,\tau,\alpha,\lambda}(t)\, l_{n,\tau}^\alpha\Big|^2\cdot\|v\|^2\,dt}\\
&= \sqrt{\int_0^\infty \Big|h_\lambda(t)-\sum_{n=0}^N s_{n,\tau,\alpha,\lambda}(t)\, l_{n,\tau}^\alpha\Big|^2\,dt}\\
&= \sqrt{\zeta(N,\tau,\alpha,\lambda)}.
\end{aligned}$$

From this inequality, it follows estimate (11).

Estimate (12) follows from Proposition 5.1 and the inequality

$$\|TDT^{-1}\|_F \leq \|T\|_{2\to2}\cdot\|D\|_F\cdot\|T^{-1}\|_{2\to2} = \varkappa(T)\cdot\|D\|_F. \quad \square$$

6 Derivatives with respect to τ

The derivatives of some of the involved functions with respect to τ have simple representations. This can help to find extreme points. In this section, we present relevant statements.

Proposition 6.1 (see [3, 4, 5]). *We have*

$$\frac{\partial l_{n,\tau}^\alpha}{\partial\tau}(t) = d_{n+1}\, l_{n+1,\tau}^\alpha(t) - d_n l_{n-1,\tau}^\alpha(t), \qquad n=0,1,\dots,$$

where $l_{-1,\tau}^\alpha(t)=0$ *and*

$$d_0=0, \qquad d_n=\frac{\sqrt{n(n+\alpha)}}{2\tau}.$$

In particular, for $\alpha=0$,

$$d_n=\frac{n}{2\tau}.$$

Proof. The proof follows from (1) and the well-known [32, formulas (5.1.14) and (5.1.10)] formulas

$$\begin{aligned}
\frac{\partial L_n^\alpha}{\partial t} &= -L_{n-1}^{\alpha+1},\\
(2n+1+\alpha-t)L_n^\alpha &= (n+1)L_{n+1}^\alpha+(n+\alpha)L_{n-1}^\alpha. \quad \square
\end{aligned}$$

Corollary 6.2. *For Laguerre coefficients* (8), *we have*

$$\frac{\partial s_{n,\tau,\alpha,\lambda}}{\partial\tau} = d_{n+1}\, s_{n+1,\tau,\alpha,\lambda} - d_n\, s_{n-1,\tau,\alpha,\lambda}, \qquad n=0,1,\dots.$$

Proof. It follows directly from (6) and Proposition 6.1. $\square$

Corollary 6.3. *For function* (9), *we have*

$$\begin{aligned}
\frac{\partial\zeta(N,\tau,\alpha,\lambda)}{\partial\tau} &= -d_{N+1}\big(s_{N+1,\tau,\alpha,\lambda}\, s_{N,\tau,\alpha,\bar\lambda} + s_{N+1,\tau,\alpha,\bar\lambda}\, s_{N,\tau,\alpha,\lambda}\big)\\
&= -2d_{N+1}\,\mathrm{Re}\big(s_{N+1,\tau,\alpha,\lambda}\, s_{N,\tau,\alpha,\bar\lambda}\big),
\end{aligned}$$

where the bar over λ *means the complex conjugate of* λ.

Proof. We make use of representation (10) and formula (7):

$$\zeta(N,\tau,\alpha,\lambda)=\sum_{n=N+1}^\infty |s_{n,\tau,\alpha,\lambda}|^2 = \sum_{n=N+1}^\infty s_{n,\tau,\alpha,\lambda}\,\overline{s_{n,\tau,\alpha,\lambda}} = \sum_{n=N+1}^\infty s_{n,\tau,\alpha,\lambda}\, s_{n,\tau,\alpha,\bar\lambda}.$$

Differentiating the last formula, we obtain

$$\frac{\partial\zeta(N,\tau,\alpha,\lambda)}{\partial\tau}=\sum_{n=N+1}^{\infty}\Big(\frac{\partial s_{n,\tau,\alpha,\lambda}}{\partial\tau}s_{n,\tau,\alpha,\bar\lambda}+s_{n,\tau,\alpha,\lambda}\frac{\partial s_{n,\tau,\alpha,\bar\lambda}}{\partial\tau}\Big).$$

Then from Corollary 6.2, it follows

$$\begin{aligned}\frac{\partial\zeta(N,\tau,\alpha,\lambda)}{\partial\tau}&=\sum_{n=N+1}^{\infty}\Big(\big(d_{n+1}s_{n+1,\tau,\alpha,\lambda}-d_n s_{n-1,\tau,\alpha,\lambda}\big)s_{n,\tau,\alpha,\bar\lambda}+s_{n,\tau,\alpha,\lambda}\big(d_{n+1}s_{n+1,\tau,\alpha,\bar\lambda}-d_n s_{n-1,\tau,\alpha,\bar\lambda}\big)\Big)\\&=\sum_{n=N+1}^{\infty}\big(d_{n+1}s_{n+1,\tau,\alpha,\lambda}s_{n,\tau,\alpha,\bar\lambda}-d_n s_{n,\tau,\alpha,\bar\lambda}s_{n-1,\tau,\alpha,\lambda}+d_{n+1}s_{n+1,\tau,\alpha,\bar\lambda}s_{n,\tau,\alpha,\lambda}-d_n s_{n,\tau,\alpha,\lambda}s_{n-1,\tau,\alpha,\bar\lambda}\big).\end{aligned}$$

After canceling we obtain the desired representation. □

7 The case $\alpha=0$

Our numerical experiments (see Section 9) show that often the optimal value of α is close to 0. For this reason, we treated the case of $\alpha=0$ as a special one in the previous exposition. In this section, we collect some additional formulas related to $\alpha=0$. These formulas and Corollary 6.3 allow one to organize calculations for the case $\alpha=0$ substantially simpler and faster than for the general case. Thus, taking α equal to 0 (though the optimal α is only close to 0), we can take a larger number N of terms in the truncated Laguerre series (5) and thereby compensate for the small loss of accuracy caused by a nonoptimal value of α.

Proposition 7.1. *Let* $\operatorname{Re}\lambda<0$*. Then the Laguerre coefficients* $s_{n,\tau,0,\lambda}$ *can be calculated recursively*:

$$\begin{aligned}s_{0,\tau,0,\lambda}&=-\frac{2\sqrt{\tau}}{2\lambda-\tau},\\s_{n+1,\tau,0,\lambda}&=\frac{2\lambda+\tau}{2\lambda-\tau}s_{n,\tau,0,\lambda}.\end{aligned}$$

Proof. It follows from Proposition 4.1. □

Corollary 7.2. *Let the spectrum of* A *lie in the left half-plane. Then the Laguerre coefficients* $S_{n,\tau,0}$ *can be calculated recursively*:

$$\begin{aligned}S_{0,\tau,0}&=-2\sqrt{\tau}(2A-\tau\mathbf{1})^{-1},\\S_{n+1,\tau,0}&=(2A+\tau\mathbf{1})(2A-\tau\mathbf{1})^{-1}S_{n,\tau,0}.\end{aligned}$$

Proof. The proof follows from Propositions 7.1 and 4.2. □

It is convenient to use Corollary 7.2 for calculating $S_{n,\tau,0}$ instead of formula (8) and Proposition 4.2 in the general case $\alpha\neq0$.

Corollary 7.3. *Let* $\operatorname{Re}\lambda<0$*. Then*

$$\begin{aligned}\zeta(N,\tau,0,\lambda)&=\frac{4\tau}{|2\lambda-\tau|^2}\cdot\frac{\left|\frac{2\lambda+\tau}{2\lambda-\tau}\right|^{2N+2}}{1-\left|\frac{2\lambda+\tau}{2\lambda-\tau}\right|^2}\\&=\frac{4\tau}{|2\lambda-\tau|^2-|2\lambda+\tau|^2}\left|\frac{2\lambda+\tau}{2\lambda-\tau}\right|^{2N+2}.\end{aligned}$$

Proof. The proof follows from formula (10) and Proposition 7.1, and the formula for the sum of the geometric series. □

8 The optimal choice of τ and α

Clearly, τ and α influence the rate of convergence of the series $\mathcal{H}=\sum_{n=0}^{\infty}S_{n,\tau,\alpha}\,l_{n,\tau}^{\alpha}$ and, consequently, the accuracy of approximation (5) for a given N. In this section, we propose an algorithm for the near-optimal choice of τ and α.

Let a stable matrix A be given. By means of the Jordan decomposition, we calculate eigenvalues and eigenvectors of A. Typically, at least due to rounding errors, the spectrum of A is simple, moreover, all eigenvalues λ_k are distinct. If the spectrum of A is not simple, the proposed algorithm for choosing τ and α also works, but less can be said about the approximation accuracy.

We take a number $N\in\mathbb{N}$. (For example, we take $N=10$.)

We consider the function

$$\varphi(N,\tau,\alpha)=\sum_{k=1}^{M}\zeta(N,\tau,\alpha,\lambda_k),$$

where λ_k are the eigenvalues of A and ζ is defined by (9).

First, we consider the case $\alpha = 0$. By Corollary 6.3, we have

$$\frac{\partial \zeta(N,\tau,0,\lambda)}{\partial \tau} = -2d_{N+1}\,\mathrm{Re}(s_{N+1,\tau,0,\lambda}\,s_{N,\tau,0,\bar{\lambda}}).$$

From Proposition 4.1 we know that

$$s_{n,\tau,0,\lambda} = -\frac{2\sqrt{\tau}(2\lambda+\tau)^n}{(2\lambda-\tau)^{n+1}}, \qquad n = 0,1,\ldots.$$

Therefore,

$$\frac{\partial \zeta(N,\tau,0,\lambda)}{\partial \tau} = -2d_{N+1}\,\mathrm{Re}\Big(\frac{2\sqrt{\tau}(2\lambda+\tau)^{N+1}}{(2\lambda-\tau)^{N+2}}\,\frac{2\sqrt{\tau}(2\bar{\lambda}+\tau)^{N}}{(2\bar{\lambda}-\tau)^{N+1}}\Big).$$

Finally, we arrive at

$$\frac{\partial \varphi(N,\tau,0)}{\partial \tau} = -2d_{N+1}\sum_{k=1}^{M}\mathrm{Re}\Big(\frac{2\sqrt{\tau}(2\lambda_k+\tau)^{N+1}}{(2\lambda_k-\tau)^{N+2}}\,\frac{2\sqrt{\tau}(2\bar{\lambda}_k+\tau)^{N}}{(2\bar{\lambda}_k-\tau)^{N+1}}\Big).$$

Numerical experiments (see Fig. 5) show that the function $\tau \mapsto \varphi(N,\tau,0)$ is convex. Hence the function $\tau \mapsto \varphi(N,\tau,0)$ has a unique minimum. We find it by solving the equation

$$\frac{\partial \varphi(N,\tau,0)}{\partial \tau} = 0$$

for τ (in 'Mathematica' [36] it is done by the command `FindRoot`; this command works iteratively; we take for the initial value $\tau = 1$). Thus, we find the optimal τ for the case $\alpha = 0$. Let us denote the optimal τ by τ_0. After that we calculate $\varphi(N,\tau_0,0)$ using Corollary 7.3 and the definition of φ.

Then we calculate symbolically $\varphi(N,\tau,\alpha)$ using formulas (8) and (10). Of course, the resulting formula is rather cumbersome. We calculate (in 'Mathematica' [36] this is done by the command `FindMinimum`)

$$\varphi_{\min}(N) = \min_{\tau>0,\,\alpha>-1}\varphi(N,\tau,\alpha).$$

We take only $N \le 12$, because the calculations are notedly slow for greater N. We take the found point of minimum (τ_1,α_1) as the optimal values of τ and α. We use $\varphi_{\min}$ for the estimates of $\|\mathcal{H} - \mathcal{H}_{N,\tau,\alpha}\|_{L_2[0,\infty)}$ according to Theorem 5.2; for the same aim, we also calculate

$$\psi(N,\tau_1,\alpha_1) = \max_{\lambda_k\in\sigma(A)}\zeta(N,\tau_1,\alpha_1,\lambda_k)$$

for the found τ_1 and α_1.

Our numerical experiments (see Section 9) show that the pair τ_0 and $\alpha_0 = 0$ is often almost optimal. So, the consideration of $\alpha \ne 0$ is not always necessary.

The proposed algorithm for finding α and τ is quite complicated and its application takes some time. If one wants to construct approximation (5) quickly, one can take rough values $\alpha = 0$ and $\tau = \|A\|/2$. The reason for such a choice of τ is as follows. We know that the spectrum $\sigma(A)$ of A is contained both in the circle of radius $\|A\|$ centered at zero and in the left half-plane. Thus, $\|A\|/2$ can be considered as the center of $\sigma(A)$.

9 Numerical experiments

In this section, we present three numerical examples.

Example 9.1. We consider the discrete model of a transmission line shown in Fig 1. We assume that the line consists of $n = 150$ sections. Thus we have 150 unknown currents I_C and 150 unknown voltages U_L. The parameters are as follows: $C = C_0/n$, $L = L_0/n$, $R = R_0/n$, $G = G_0/n$, where $C_0 = 10$, $L_0 = 50$, $R_0 = 170$, $G_0 = 160$. The state variable [34] description of the circuit has the form $\dot{x}(t) = Ax(t) + f(t)$ with a matrix A of the size 300×300. The spectrum of $-A$ is shown in Fig. 2.

First, we consider the case of the simplest choice of α and τ. We set $\alpha = 0$. We calculate $\|A\|_{1\to1} = 33.2$, where $\|A\|_{1\to1}$ is the norm of the matrix A induced by the norm $\|x\|_1 = |x_1| + |x_2| + \ldots + |x_M|$ on $\mathbb{C}^M$. Then we take the heuristic (simplified) value $\tau_* = \|A\|_{1\to1}/2 = 16.6$. Such a quick choice of α and τ allows to apply formulas from Corollary 7.2 to construct approximation (5) immediately; we consider two cases: $N = 10$ and $N = 30$ in the truncated Laguerre series (5). Using Theorem 5.2 we obtain the estimates (we recall that to obtain the estimates, it is necessary to calculate the eigendecomposition and $\varkappa(T) = 28.358$)

$$\|\mathcal{H} - \mathcal{H}_{10,\tau_*,0}\|_{L_2[0,\infty)} \ge \sqrt{\psi(10,\tau_*,0)} = 0.00024,$$
$$\|\mathcal{H} - \mathcal{H}_{10,\tau_*,0}\|_{L_2[0,\infty)} \le \varkappa(T)\sqrt{\varphi(10,\tau_*,0)} = 0.0476,$$
$$\|\mathcal{H} - \mathcal{H}_{30,\tau_*,0}\|_{L_2[0,\infty)} \ge \sqrt{\psi(30,\tau_*,0)} = 9.27\cdot10^{-10},$$
$$\|\mathcal{H} - \mathcal{H}_{30,\tau_*,0}\|_{L_2[0,\infty)} \le \varkappa(T)\sqrt{\varphi(30,\tau_*,0)} = 1.44\cdot10^{-6}.$$

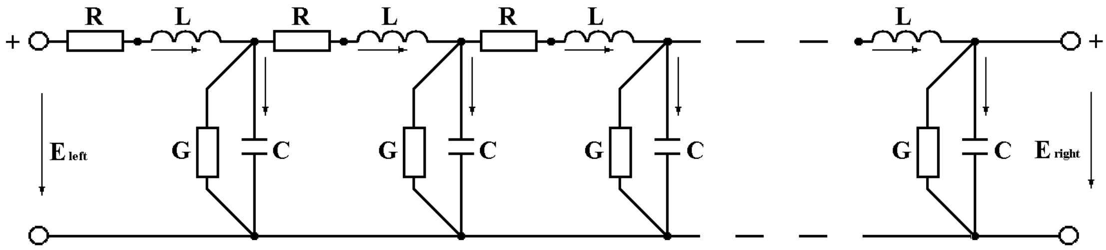

Figure 1: A discrete model of a transmission line

Second, we take $\alpha = 0$ and $N = 10$. Then we calculate the minimum of φ over τ; as the initial value of τ (for the iteratively finding the minimum) we take $\tau = 1$. We obtain the following results (left Fig. 2). The optimal τ is $\tau_0 = 19.196$ (it is shown in the left Fig. 2 as a small square). According to Theorem 5.2 we have

$$\|\mathcal{H} - \mathcal{H}_{10,\tau_0,0}\|_{L_2[0,\infty)} \geq \sqrt{\psi(10,\tau_0,0)} = 0.000192,$$
$$\|\mathcal{H} - \mathcal{H}_{10,\tau_0,0}\|_{L_2[0,\infty)} \leq \varkappa(T)\sqrt{\varphi(10,\tau_0,0)} = 0.0294.$$

After that, we repeat the same experiment with $N = 30$. We obtain $\tau_0 = 19.3$ and

$$\|\mathcal{H} - \mathcal{H}_{30,\tau_0,0}\|_{L_2[0,\infty)} \geq \sqrt{\psi(30,\tau_0,0)} = 2.07 \cdot 10^{-10},$$
$$\|\mathcal{H} - \mathcal{H}_{30,\tau_0,0}\|_{L_2[0,\infty)} \leq \varkappa(T)\sqrt{\varphi(30,\tau_0,0)} = 2.47 \cdot 10^{-8}.$$

Third, we return to $N = 10$, take as initial values the found $\tau_0 = 19.2$ and $\alpha = 0$, and find the minimum of $\varphi(N,\tau,\alpha)$ over τ and α. We obtain the following results (right Fig. 2). The optimal τ is $\tau_1 = 19.201$; the optimal α is $\alpha_1 = 0.0000239$. According to Theorem 5.2 we have

$$\|\mathcal{H} - \mathcal{H}_{10,\tau_1,\alpha_1}\|_{L_2[0,\infty)} \geq \sqrt{\psi(10,\tau_1,\alpha_1)} = 0.000193,$$
$$\|\mathcal{H} - \mathcal{H}_{10,\tau_1,\alpha_1}\|_{L_2[0,\infty)} \leq \varkappa(T)\sqrt{\varphi(10,\tau_1,\alpha_1)} = 0.0294.$$

Thus, we have practically the same result as for $\alpha = 0$.

To show the actual convergence rate and the difference between the Frobenius norm and the usual norm, we calculate the coefficients $S_{n,\tau,\alpha}$ according to Propositions 4.1, 4.2 and Corollary 7.2 for two cases: $\tau_0 = 19.196$, $\alpha_0 = 0$ and $\tau_1 = 19.201$, $\alpha_1 = 0.0000239$. Then we calculate the norms of the coefficients $S_{n,\tau,\alpha}$. The results for these two cases coincide to within 6 significant digits. Therefore, we present the results only for the first case, see Table 1. We see that the difference between the Frobenius norm $\|\cdot\|_F$ and the norm $\|\cdot\|_{2\to2}$ induced by the Euclidean norm on $\mathbb{C}^M$ is not high.

Table 1: The norms of the coefficients $S_{n,19.2,0}$

n	0	1	2	3	4	5	6	7	8	9
$\|S_{n,19.2,0}\|_F$	4.54	2.28	1.13	0.378	0.171	0.114	0.0435	0.0177	0.0127	0.00538
$\|S_{n,19.2,0}\|_{2\to2}$	0.351	0.199	0.135	0.0494	0.0214	0.017	0.00702	0.00267	0.00211	0.000979

n	10	11	12	13	14	15	16	17
$\|S_{n,19.2,0}\|_F$	0.00195	0.00146	0.000679	0.000227	0.000168	0.0000861	2.79×10^{-5}	1.94×10^{-5}
$\|S_{n,19.2,0}\|_{2\to2}$	0.000334	0.000257	0.000134	0.0000417	0.0000308	0.000018	5.22×10^{-6}	3.62×10^{-6}

n	18	19	20	21	22	23
$\|S_{n,19.2,0}\|_F$	1.09×10^{-5}	3.56×10^{-6}	2.23×10^{-6}	1.37×10^{-6}	4.7×10^{-7}	2.55×10^{-7}
$\|S_{n,19.2,0}\|_{2\to2}$	2.38×10^{-6}	6.92×10^{-7}	4.18×10^{-7}	3.1×10^{-7}	1.02×10^{-7}	4.72×10^{-8}

n	24	25	26	27	28	29
$\|S_{n,19.2,0}\|_F$	1.71×10^{-7}	6.28×10^{-8}	2.92×10^{-8}	2.12×10^{-8}	8.44×10^{-9}	3.38×10^{-9}
$\|S_{n,19.2,0}\|_{2\to2}$	3.96×10^{-8}	1.47×10^{-8}	5.23×10^{-9}	4.99×10^{-9}	2.09×10^{-9}	6.36×10^{-10}

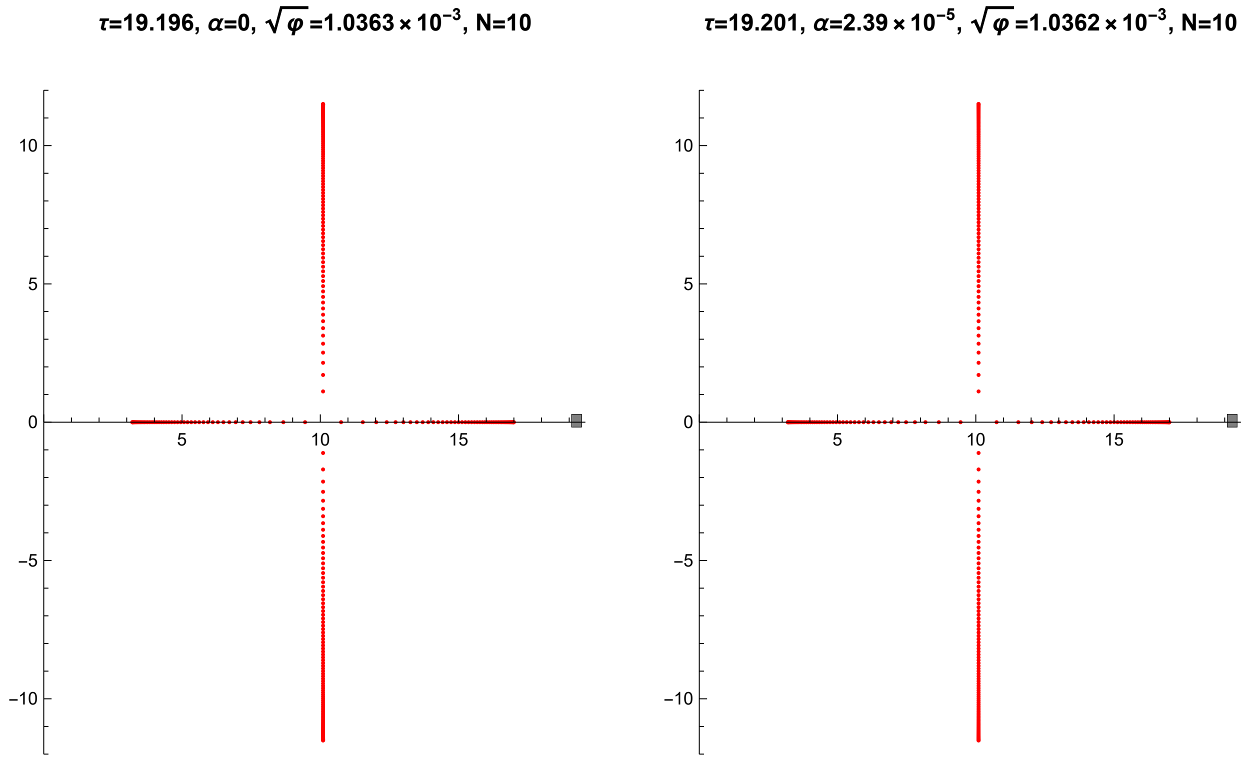

Figure 2: The points show the spectrum of the matrix $-A$ from example 9.1, the small squares are the found τ. In the right figure the minimum is taken over τ and α; in the left figure the minimum is taken only over τ with $\alpha = 0$

Example 9.2. We consider the matrix

$$A = -\begin{pmatrix} a_{M-1} & a_{M-2} & \dots & a_1 & a_0 \\ 1 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 \end{pmatrix} - 1.1 \begin{pmatrix} 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 1 \end{pmatrix}$$

of the size $M \times M$ with $M = 500$, where a_i are random numbers uniformly distributed in $[0, 1]$. The matrix A is a type of so-called companion matrix that occurs in differential equations [13, p. 528]. The spectrum of A is close to a circumference of radius 1 (to make the matrix stable, we subtract $1.1 \cdot \mathbf{1}$), see Fig 3.

First, we consider the case of the simplest choice of α and τ. We set $\alpha = 0$. We calculate $\|A\|_{1\to1} = 3.1$, where $\|A\|_{1\to1}$ is the norm of the matrix A induced by the norm $\|x\|_1 = |x_1| + |x_2| + \ldots + |x_M|$ on $\mathbb{C}^M$. Then we take the heuristic (simplified) value $\tau_* = \|A\|_{1\to1}/2 = 1.55$. Such a quick choice of α and τ allows to apply formulas from Corollary 7.2 to construct approximation (5) immediately; we consider two cases: $N = 10$ and $N = 30$ in the truncated Laguerre series (5). Using Theorem 5.2 we obtain the estimates (we recall that to obtain the estimates, it is necessary to calculate the eigendecomposition; in this case $\varkappa(T) = 44.54$)

$$\|\mathcal{H} - \mathcal{H}_{10,\tau_*,0}\|_{L_2[0,\infty)} \geq \sqrt{\psi(10, \tau_*, 0)} = 0.253,$$
$$\|\mathcal{H} - \mathcal{H}_{10,\tau_*,0}\|_{L_2[0,\infty)} \leq \varkappa(T)\sqrt{\varphi(10, \tau_*, 0)} = 32.76,$$
$$\|\mathcal{H} - \mathcal{H}_{30,\tau_*,0}\|_{L_2[0,\infty)} \geq \sqrt{\psi(30, \tau_*, 0)} = 0.00393,$$
$$\|\mathcal{H} - \mathcal{H}_{30,\tau_*,0}\|_{L_2[0,\infty)} \leq \varkappa(T)\sqrt{\varphi(30, \tau_*, 0)} = 0.233.$$

Second, we set $\alpha = 0$. Since we know the form of the spectrum, now we take another heuristic value $\tau_{**} = 1$. We consider

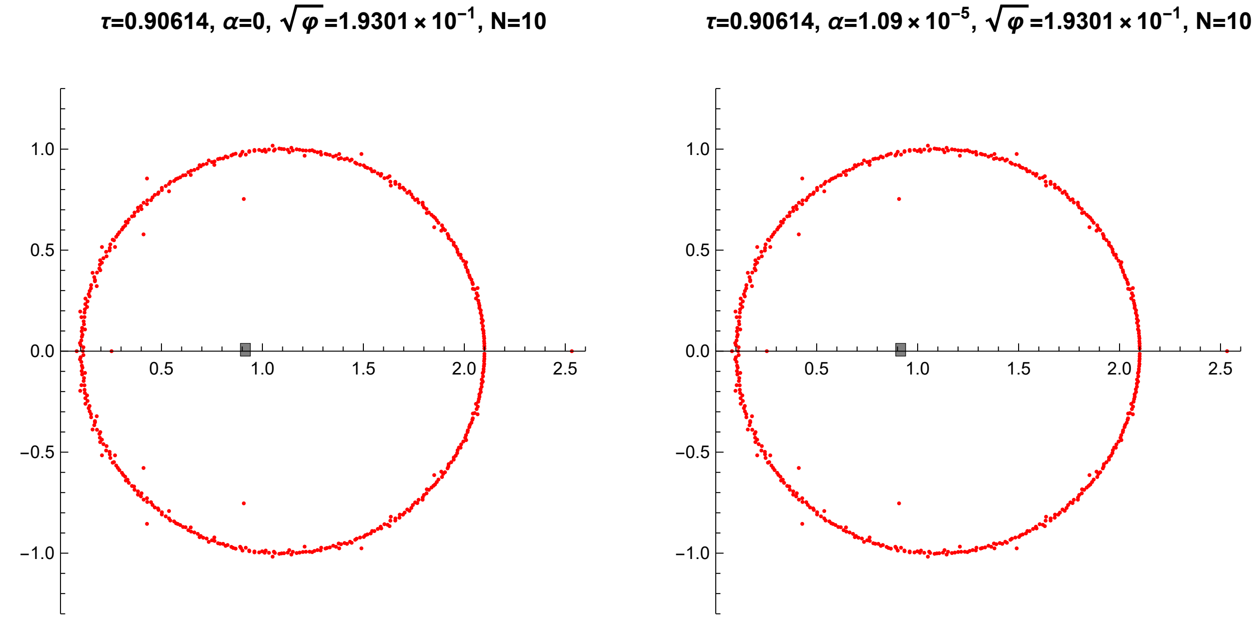

Figure 3: The points show the spectrum of the matrix $-A$ from example 9.2, the small squares are the found τ. In the right figure the minimum is taken over τ and α; in the left figure the minimum is taken only over τ with $\alpha = 0$. The results coincide within 5 significant digits

two cases: $N = 10$ and $N = 30$ in the truncated Laguerre series (5). Using Theorem 5.2 we obtain the estimates

$$\|\mathcal{H} - \mathcal{H}_{10,\tau_{**},0}\|_{L_2[0,\infty)} \geq \sqrt{\psi(10,\tau_{**},0)} = 0.0705,$$
$$\|\mathcal{H} - \mathcal{H}_{10,\tau_{**},0}\|_{L_2[0,\infty)} \leq \varkappa(T)\sqrt{\varphi(10,\tau_{**},0)} = 9.54,$$
$$\|\mathcal{H} - \mathcal{H}_{30,\tau_{**},0}\|_{L_2[0,\infty)} \geq \sqrt{\psi(30,\tau_{**},0)} = 0.000107,$$
$$\|\mathcal{H} - \mathcal{H}_{30,\tau_{**},0}\|_{L_2[0,\infty)} \leq \varkappa(T)\sqrt{\varphi(30,\tau_{**},0)} = 0.0065.$$

Third, we take $\alpha = 0$ and $N = 10$. Then we calculate the minimum of φ over τ; as the initial value of τ we take $\tau = 1$. We obtain the following results (left Fig. 3). The optimal τ is $\tau_0 = 0.906$ (it is shown in the left Fig. 3 as a small square). According to Theorem 5.2 we have

$$\|\mathcal{H} - \mathcal{H}_{10,\tau_0,0}\|_{L_2[0,\infty)} \geq \sqrt{\psi(10,\tau_0,0)} = 0.048,$$
$$\|\mathcal{H} - \mathcal{H}_{10,\tau_0,0}\|_{L_2[0,\infty)} \leq \varkappa(T)\sqrt{\varphi(10,\tau_0,0)} = 8.6.$$

After that, we repeat the same experiment with $N = 30$. We obtain $\tau_0 = 0.875$ and

$$\|\mathcal{H} - \mathcal{H}_{30,\tau_0,0}\|_{L_2[0,\infty)} \geq \sqrt{\psi(30,\tau_0,0)} = 0.0000246,$$
$$\|\mathcal{H} - \mathcal{H}_{30,\tau_0,0}\|_{L_2[0,\infty)} \leq \varkappa(T)\sqrt{\varphi(30,\tau_0,0)} = 0.0027.$$

Fourth, we return to $N = 10$, take as initial values the found $\tau_0 = 19.2$ and $\alpha = 0$, and find the minimum of $\varphi(N,\tau,\alpha)$ over τ and α. We obtain the following results (right Fig. 3). The optimal τ is $\tau_1 = 0.906$; the optimal α is $\alpha_1 = 0.000011$. According to Theorem 5.2 we have

$$\|\mathcal{H} - \mathcal{H}_{10,\tau_1,\alpha_1}\|_{L_2[0,\infty)} \geq \sqrt{\psi(10,\tau_1,\alpha_1)} = 0.048,$$
$$\|\mathcal{H} - \mathcal{H}_{10,\tau_1,\alpha_1}\|_{L_2[0,\infty)} \leq \varkappa(T)\sqrt{\varphi(10,\tau_1,\alpha_1)} = 8.6.$$

Thus, we have practically the same result as for $\alpha = 0$.

Example 9.3. In Examples 9.1 and 9.2 the minimum of $\varphi(N,\tau,\alpha)$ is attained almost at $\alpha = 0$. We present here another example of the same kind. Since the point of minimum in our estimate depends only on the spectrum of A, we do not present a matrix A itself and work only with its possible spectrum.

We take 3000 random complex numbers; their real parts have the Maxwell distribution with $\sigma = 4$ (the probability density for value x in the Maxwell distribution is proportional to $x^2 e^{-x^2/(2\sigma^2)}$ for $x > 0$, and is zero for $x < 0$; the use of the Maxwell distribution here is not related to any special application, we just want to have a random distribution in the complex left half-plane) and imaginary parts have the normal distribution with the mean value $\mu = 0$ and the variance $\sigma^2 = 1$. We interpret these points as a possible spectrum of $-A$; we present them in Fig. 4. The results of calculation are as follows.

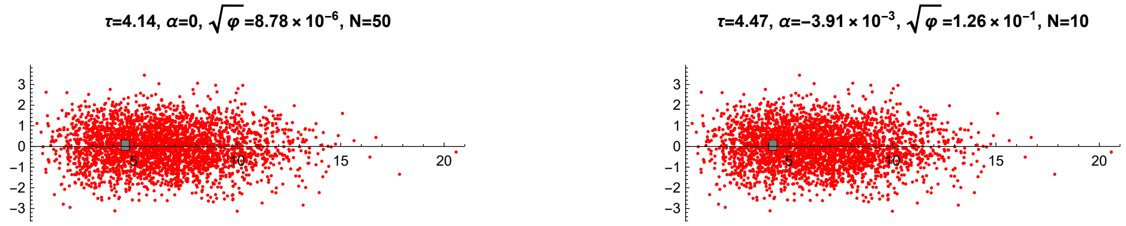

Figure 4: The points from Example 9.3, the small squares are the found τ. In the right figure the minimum is taken over τ and α; in the left figure the minimum is taken only over τ with $\alpha = 0$. Note that in the right fig. $N = 10$, but in the left fig. $N = 50$

.

First we take $N = 10$ and $\alpha = 0$. Starting from the initial point $\tau = 1$, we find that the minimum of $\varphi(10, \tau, 0)$ over τ is attained at $\tau_0 = 4.50$ and

$$\sqrt{\varphi(10, \tau_0, 0)} = 0.1269,$$
$$\sqrt{\psi(10, \tau_0, 0)} = 0.1040.$$

The experiment with $N = 30$ and $\alpha = 0$ gives $\tau_0 = 3.97$ and

$$\sqrt{\varphi(30, \tau_0, 0)} = 0.00085,$$
$$\sqrt{\psi(30, \tau_0, 0)} = 0.00067.$$

The experiment with $N = 50$ and $\alpha = 0$ gives $\tau_0 = 4.14$ and

$$\sqrt{\varphi(30, \tau_0, 0)} = 8.77 \cdot 10^{-6},$$
$$\sqrt{\psi(30, \tau_0, 0)} = 6.87 \cdot 10^{-6}.$$

Then again we take $N = 10$ and find the minimum of $\varphi(N, \tau, \alpha)$ over τ and α (we begin iterations from the found $\tau_0 = 4.50$ and $\alpha = 0$). Now the optimal τ is $\tau_1 = 4.47$ and the optimal α is $\alpha_1 = -0.0039$. For the estimates from Theorem 5.2 we have

$$\sqrt{\varphi(10, \tau_1, \alpha_1)} = 0.1259,$$
$$\sqrt{\psi(10, \tau_1, \alpha_1)} = 0.1027.$$

Fig. 5 shows that the function $\sqrt{\varphi}$ is rather smooth and convex. Thus, the problem of finding of its minimum can be solved by standard tools.

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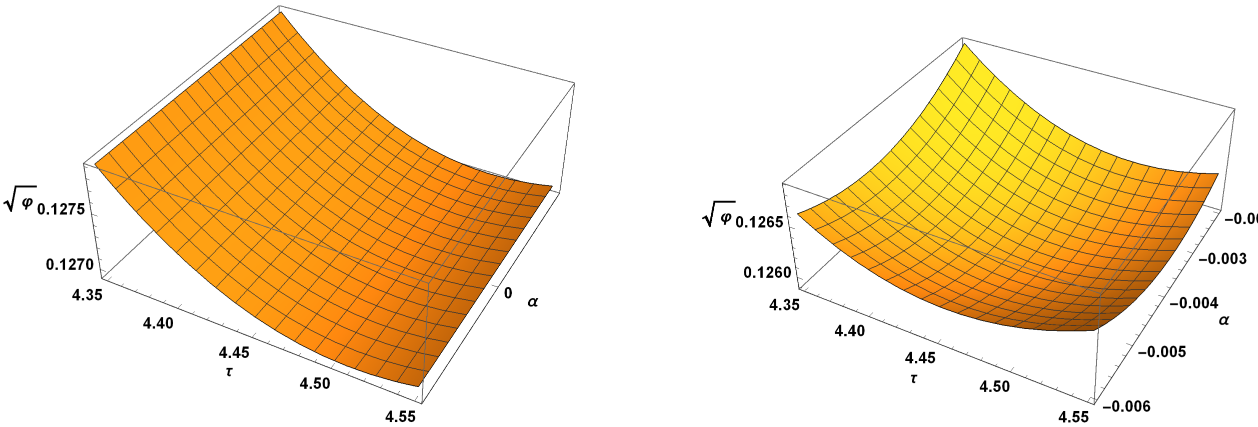

Figure 5: The graphs of the function $\sqrt{\varphi}$ from Examples 9.3 at constant $\alpha = 0$ (left) and with changing α (right) for $N = 10$ in a neighbourhood of the minimum point

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