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# Improvement on the bound of Hermite matrix polynomials ☆

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ABSTRACT

In this paper, we introduce an improved bound on the 2-norm of Hermite matrix polynomials. As a consequence, this estimate enables us to present and prove a matrix version of the Riemann–Lebesgue lemma for Fourier transforms. Finally, our theoretical results are used to develop a novel procedure for the computation of matrix exponentials with *a priori* bounds. A numerical example for a test matrix is provided.



## 1. Introduction

Orthogonal matrix polynomials emerge in various important areas of applied mathematics. In previous work, an extension of the classical family of Hermite polynomials to the matrix framework has been proposed [8]. Later on some essential properties of series expansions of Hermite matrix polynomials and their bounds were shown [2,3]. Only very recently, new extensions of Hermite matrix polynomials have been given in the literature, see *e.g.* [1,14].

The principal aim of this paper is to provide some answers to problems arising in the study of the expansions of matrix functions in terms of Hermite matrix polynomials $H_n(x, A)$. In particular, a new bound on their Euclidean norm $\|H_n(x, A)\|_2$ is derived. This new bound not only improves considerably

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upon previously established estimates of Ref. [2], but also permits to prove that the Fourier coefficients corresponding to the Hermite matrix polynomials $H_n(x, A)$ vanish when $n \to \infty$, which previously was not possible.

Subsequently a matrix analogue of the Riemann–Lebesgue lemma for a sequence of Hermite matrix polynomials is proven. Then, this new bound is used to compute matrix exponential approximations with a predetermined accuracy.

The organization of the paper is as follows: in Section 2, the matrix functional associated to Hermite matrix polynomials is defined in an appropriate Banach space, whose norm is related to the matrix functional. Unlike the scalar case, the norm in the Banach space of matrix functions does not require a Hilbert structure. Section 3 contains the explicit derivation of the new bound on $\|H_n(x, A)\|_2$ and demonstrates how this bound is used to obtain a matrix version of the Riemann–Lebesgue lemma. Finally, a numerical example follows to illustrate a new method to compute the matrix exponential, which is based on this lemma.

Throughout this paper, a matrix polynomial of degree $n$ in $\mathbb{C}^{r\times r}$ is denoted by $P(x) = A_n x^n + A_{n-1}x^{n-1} + \cdots + A_1 x + A_0$, where $x \in \mathbb{R}$, and $A_j \in \mathbb{C}^{r\times r}$ represents a complex square matrix for $0 \leqslant j \leqslant n$. Also, the set of all matrix polynomials in $\mathbb{C}^{r\times r}$, for all $n \geqslant 0$, will be given by $\mathcal{P}[x]$. Further, let $f(z)$ and $g(z)$ be holomorphic functions of the complex variable $z$, which are defined in an open set $\Omega$ of the complex plane. If $C$ is a matrix in $\mathbb{C}^{r\times r}$ so that the set of all its eigenvalues, $\sigma(C)$, lies in $\Omega$, then, from the properties of the matrix functional calculus [5, p. 558], it follows that

$$f(C)g(C) = g(C)f(C). \tag{1}$$

As usual, the 2-norm of a matrix $C \in \mathbb{C}^{r\times r}$ is defined by (see [7, p. 56]):

$$\|C\|_2 = \sup_{x\neq 0} \frac{\|Cx\|_2}{\|x\|_2},$$

where for a vector $y$ in $\mathbb{C}^r$, $\|y\|_2$ denotes the ordinary Euclidean norm. Using the matrix components $C = (c_{ij})_{1\leqslant i,j\leqslant r}$, by Golub and van Loan [7, p. 57] one obtains

$$\max_{1\leqslant i,j\leqslant r} |c_{ij}| \leqslant \|C\|_2 \leqslant r \max_{1\leqslant i,j\leqslant r} |c_{ij}|. \tag{2}$$

For an estimation on the bound of the exponential matrix, we introduce the real value $\beta(A) = \min\{\mathrm{Re}(z);\, z \in \sigma(A)\}$. Then, by [6, p. 336, 556] it follows that

$$\left\| e^{-A\,t^2} \right\|_2 \leqslant e^{-\beta(A)t^2} M^A_{r-1}(t^2), \quad \text{with } t \geqslant 0, \tag{3}$$

where $M^A_{r-1}(t^2)$ is defined by the following expansion

$$M^A_{r-1}(t^2) = \sum_{k=0}^{r-1} \frac{\left(\|A\|_2\sqrt{r}t^2\right)^k}{k!}.$$

If $\mathbb{D}_0$ is the complex plane cut along the negative real axis, and $\log(z)$ denotes the principal logarithm of $z$, [11, p. 72], then $z^{\frac{1}{2}}$ represents $\exp\left(\frac{1}{2}\log(z)\right)$.

If $B$ is a matrix with $\sigma(B) \subset \mathbb{D}_0$, then $B^{\frac{1}{2}} = \sqrt{B}$ denotes the image of $z^{\frac{1}{2}}$ of the matrix functional calculus acting on the matrix $B$. We say that matrix $A$ in $\mathbb{C}^{r\times r}$ is a positive stable matrix if $\mathrm{Re}(z) > 0$ for all $z \in \sigma(A)$. For a positive stable matrix $A$ in $\mathbb{C}^{r\times r}$, the $n$th Hermite matrix polynomial is defined by Jódar and Company [8]

$$H_n(x, A) = n! \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{(-1)^k \left(\sqrt{2A}\right)^{n-2k}}{k!(n-2k)!} x^{n-2k}, \tag{4}$$

where $\lfloor x \rfloor$ is the standard floor function which maps a real number $x$ to its next smallest integer. Furthermore, we will also use the analogous ceiling function $\lceil x \rceil$, producing the next largest integer to $x \in \mathbb{R}$.

Note also that if $A(k, n)$ is a matrix in $\mathbb{C}^{r\times r}$ for $n \geqslant 0$, $k \geqslant 0$, one may use the following identity [3]:

$$\sum_{n\geqslant 0}\sum_{k\geqslant 0} A(k, n) = \sum_{n\geqslant 0}\sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} A(k, n-2k). \tag{5}$$

In what follows, *integrable* will always imply integrable in the Lebesgue sense.

## 2. Some preliminaries on Hermite matrix polynomials and Hermite matrix functionals

Let $A$ be a positive stable matrix in $\mathbb{C}^{r\times r}$. Then, $L_A^2(\mathbb{R}, \mathbb{C}^{r\times r})$ is the vector space for all $\mathbb{C}^{r\times r}$ valued functions $f : \mathbb{R} \to \mathbb{C}^{r\times r}$ such that

$$\int_{-\infty}^{+\infty} \|f(x)\|_2^2 \, e^{-\frac{\beta(A)x^2}{2}} dx < \infty,$$

and is endowed with the norm

$$\|f\| = \left\{ \int_{-\infty}^{+\infty} \|f(x)\|_2^2 \, e^{-\frac{\beta(A)x^2}{2}} dx \right\}^{\frac{1}{2}}. \tag{6}$$

Notice that the scalar functions $h(x)$, having an appropriately normed space, may be defined to possess the following Banach structure

$$L_A^2(\mathbb{R}, \mathbb{C}) = \left\{ h : \mathbb{R} \to \mathbb{C};\ \int_{-\infty}^{+\infty} |h(x)|^2 \, e^{-\frac{\beta(A)x^2}{2}} dx < \infty \right\},$$

with the norm [6]

$$\|h\|_2 = \left\{ \int_{-\infty}^{+\infty} |h(x)|^2 \, e^{-\frac{\beta(A)x^2}{2}} dx < \infty \right\}^{\frac{1}{2}}.$$

Taking also into account the limits given in Eq. (2), it is straightforward to see that the space $L_A^2(\mathbb{R}, \mathbb{C}^{r\times r})$ is likewise a Banach space. The Banach structure of scalar functions essentially induces the Banach structure of the matrix case with the 2-norm of Eq. (6).

We are now in the position to introduce the Hermite matrix functional $\mathcal{L} : L_A^2(\mathbb{R}, \mathbb{C}^{r\times r}) \times L_A^2(\mathbb{R}, \mathbb{C}^{r\times r}) \to \mathbb{C}^{r\times r}$ defined by

$$\mathcal{L}(f, g) = \int_{-\infty}^{+\infty} f(x)\, e^{-\frac{Ax^2}{2}} g(x)\, dx. \tag{7}$$

Thus, the following properties of $\mathcal{L}$ are obvious:

(i) $\mathcal{L}(Pf, g) = P\mathcal{L}(f, g)$, $\quad \mathcal{L}(f, gP) = \mathcal{L}(f, g)P$, $\quad$ for $P \in \mathbb{C}^{r\times r}$;

(ii) $\mathcal{L}(f + g, h) = \mathcal{L}(f, h) + \mathcal{L}(g, h)$, $\quad \mathcal{L}(f, g + h) = \mathcal{L}(f, g) + \mathcal{L}(f, h)$, for $f, g, h \in L_A^2(\mathbb{R}, \mathbb{C}^{r\times r})$.

By applying the commutation property Eq. (1) to the Hermite matrix polynomials sequence $\{H_n(\cdot, A)\}_{n \geqslant 0}$, one readily obtains

$$\mathcal{L}\left(H_n(\cdot, A), H_m(\cdot, A)\right) = \mathcal{L}\left(H_m(\cdot, A), H_n(\cdot, A)\right),$$

and by Ref. [8, Eqs. (4.4) and (4.9)], it follows that

$$\mathcal{L}\left(H_n(\cdot, A), H_m(\cdot, A)\right) = 0, \text{ for } n \neq m,$$

and also

$$\mathcal{L}\left(H_n(\cdot, A), H_n(\cdot, A)\right) = 2^n n! \left(2\pi A^{-1}\right)^{\frac{1}{2}}, \text{ for } n \geqslant 0.$$

Therefore, the sequence $\{H_n(\cdot, A)\}_{n \geqslant 0}$ specifies a sequence of orthogonal matrix polynomials in $L_A^2\left(\mathbb{R}, \mathbb{C}^{r\times r}\right)$ with respect to $\mathcal{L}$ [4].

## 3. A new bound for Hermite matrix polynomials

The primary purpose of this paper is to develop an upper bound on $\|H_n(x, A)\|_2$. The bound will be given in Theorem 1. As an immediate application, we can deduce a matrix version of the Riemann–Lebesgue lemma, which would be impossible to prove with previously published bounds, as *e.g.* Ref. [2]. Another direct application is the design of a novel algorithm for computing $e^A$, where $A$ is any $r \times r$ matrix. This computational scheme, in fact, has the advantage of complying with an arbitrary approximation error condition which may be prescribed *a priori*.

**Theorem 1.** *If $A \in \mathbb{C}^{r\times r}$ is a positive stable matrix, then*

$$\|H_n(x, A)\|_2 \leqslant n!\, e^{\left(|x| \left\|\sqrt{2A}\right\|_2 + 1\right)}, \quad \forall\, x \in \mathbb{R}, n \geqslant 0. \tag{8}$$

**Proof.** Taking the norm of Eq. (4), one finds

$$\|H_n(x, A)\|_2 \leqslant n! \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{\left(|x| \left\|\sqrt{2A}\right\|_2\right)^{n-2k}}{k!(n-2k)!}. \tag{9}$$

On the other hand, applying the summation rule (5), it follows that

$$\begin{aligned} e^{|x| \left\|\sqrt{2A}\right\|_2 + 1} &= \sum_{n \geqslant 0} \frac{\left(|x| \left\|\sqrt{2A}\right\|_2\right)^n}{n!} \sum_{k \geqslant 0} \frac{1}{k!} = \sum_{n \geqslant 0} \sum_{k \geqslant 0} \frac{\left(|x| \left\|\sqrt{2A}\right\|_2\right)^n}{k!n!} \\ &= \sum_{n \geqslant 0} \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{\left(|x| \left\|\sqrt{2A}\right\|_2\right)^{n-2k}}{k!(n-2k)!}. \end{aligned} \tag{10}$$

And consequently it is

$$\sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{\left(|x| \left\|\sqrt{2A}\right\|_2\right)^{n-2k}}{k!(n-2k)!} \leqslant e^{|x| \left\|\sqrt{2A}\right\|_2 + 1}, \tag{11}$$

which by Eqs. (9)–(11) proves Eq. (8). $\square$

It is noteworthy to mention that our matrix bound Eq. (8) for $r = 1$ and $A = 2$ reduces to the following expression

$$|H_n(x)| \leqslant n!\, e^{2|x|+1}, \quad \forall\, x \in \mathbb{R}, n \geqslant 0,$$

because in this case the Hermite matrix polynomials Eq. (4) coincide with the standard Hermite polynomials. This formula is similar to the scalar expression derived by Cramer who found the bound:

$$|H_n(x)| \leqslant k\sqrt{n!}\, 2^{n/2} e^{x^2/2}, \quad \forall\, x \in \mathbb{R}, n \geqslant 0,$$

with constant $k = 1.086435$, see [12, p. 324].

### 3.1. A theoretical application: proof of a Riemann–Lebesgue matrix lemma

Following the procedure presented in Ref. [13], the $k$th left matrix Fourier coefficient of $f \in L^2_A(\mathbb{R}, \mathbb{C}^{r\times r})$ with respect to $\{H_n(\cdot, A)\}_{n\geqslant 0}$ is introduced by

$$\begin{aligned} C_k(f) &= \frac{1}{\sqrt{2\pi}\, 2^k k!}\, \mathcal{L}(f, H_k(\cdot, A))A^{\frac{1}{2}} \\ &= \frac{1}{\sqrt{2\pi}\, 2^k k!} \left(\int_{-\infty}^{+\infty} f(t)\, e^{-\frac{At^2}{2}} H_k(t, A)\, dt\right) A^{\frac{1}{2}}, \end{aligned} \tag{12}$$

and the corresponding left Fourier series of $f \in L^2_A(\mathbb{R}, \mathbb{C}^{r\times r})$ with respect to $\{H_n(\cdot, A)\}_{n\geqslant 0}$ is then defined by

$$S(f)(x) = \sum_{n\geqslant 0} C_n(f) H_n(x, A).$$

Our aim is to show that $\lim_{n\to\infty} C_n(f) = 0$. First, we can observe that by using Eq. (12), it follows that

$$\|C_n(f)\|_2 \leqslant \frac{\left\|A^{\frac{1}{2}}\right\|_2}{\sqrt{2\pi}\, 2^n n!} \int_{-\infty}^{+\infty} \|f(t)\|_2 \left\|e^{-\frac{A}{2}t^2}\right\|_2 \|H_n(t, A)\|_2\, dt. \tag{13}$$

Taking into account the estimate Eq. (3) and substituting Eq. (8) into Eq. (13), one finds by using the Cauchy–Schwarz inequality:

$$\begin{aligned} \|C_n(f)\|_2 &\leqslant \frac{\left\|A^{\frac{1}{2}}\right\|_2 e}{\sqrt{2\pi}\, 2^n} \sum_{k=0}^{r-1} \frac{\left(\|A\|_2\sqrt{r}\right)^k}{k!} \int_{-\infty}^{+\infty} \|f(t)\|_2\, e^{-\frac{\beta(A)}{2}t^2} t^{2k} e^{|t|\,\left\|\sqrt{2A}\right\|_2} dt \\ &= \frac{\left\|A^{\frac{1}{2}}\right\|_2 e}{\sqrt{2\pi}\, 2^n} \sum_{k=0}^{r-1} \frac{\left(\|A\|_2\sqrt{r}\right)^k}{k!} \left(\int_{-\infty}^{+\infty} \|f(t)\|_2^2\, e^{-\frac{\beta(A)}{2}t^2} dt\right)^{\frac{1}{2}} \\ &\quad \times \left(\int_{-\infty}^{+\infty} e^{-\frac{\beta(A)}{2}t^2} e^{2|t|\,\left\|\sqrt{2A}\right\|_2} t^{4k} dt\right)^{\frac{1}{2}} \\ &= \frac{\left\|A^{\frac{1}{2}}\right\|_2 e\, \|f\|}{\sqrt{2\pi}\, 2^n} \sum_{k=0}^{r-1} \frac{\left(\|A\|_2\sqrt{r}\right)^k}{k!} \left(\int_{-\infty}^{+\infty} e^{-\frac{\beta(A)}{2}t^2} e^{2|t|\left\|\sqrt{2A}\right\|_2} t^{4k} dt\right)^{\frac{1}{2}}, \end{aligned}$$

since $\left(\int_{-\infty}^{+\infty} \|f(t)\|_2^2\, e^{-\frac{\beta(A)}{2}t^2} dt\right)^{\frac{1}{2}} = \|f\|$ by Eq. (6). Furthermore, we can simplify

$$\|C_n(f)\|_2 \leqslant \frac{2\left\|A^{\frac{1}{2}}\right\| e\|f\|_2}{\sqrt{2\pi}2^n} \sum_{k=0}^{r-1} \frac{\left(\|A\|_2 \sqrt{r}\right)^k}{k!} \left(\int_0^{+\infty} e^{-\frac{\beta(A)}{2}t^2} e^{2t\left\|\sqrt{2A}\right\|_2} t^{4k} dt\right)^{\frac{1}{2}}$$
$$\leqslant \frac{\left\|A^{\frac{1}{2}}\right\|_2 e\|f\|R}{\sqrt{2\pi}2^{n-1}} \sum_{k=0}^{r-1} \frac{\left(\|A\|_2 \sqrt{r}\right)^k}{k!},$$

where $R = \max\left\{\left(\int_0^{+\infty} e^{-\frac{\beta(A)}{2}t^2} e^{2t\left\|\sqrt{2A}\right\|_2} t^{4k} dt\right)^{\frac{1}{2}}; k = 0, 1, \ldots, r-1\right\}$, and hence it follows that $\lim_{n\to\infty} C_n(f) = 0$.

In conclusion, the following result has been demonstrated:

**Theorem 2** (Matrix Riemann–Lebesgue property)**.** *Let $\mathcal{L}$ be the Hermite matrix functional on $L_A^2(\mathbb{R}, \mathbb{C}^{r\times r})$ defined by Eq. (7). If $f \in L_A^2(\mathbb{R}, \mathbb{C}^{r\times r})$, then it follows that $\lim_{n\to\infty} C_n(f) = 0$.*

**Remark 1.** Following again Ref. [13], the $k$th right matrix Fourier coefficient of $f \in L_A^2(\mathbb{R}, \mathbb{C}^{r\times r})$ with respect to $\{H_n(\cdot, A)\}_{n\geqslant 0}$, is denoted by

$$C_k(f) = \frac{A^{\frac{1}{2}}}{\sqrt{2\pi}2^k k!}\mathcal{L}(H_k(\cdot, A), f) = \frac{A^{\frac{1}{2}}}{\sqrt{2\pi}2^k k!}\left(\int_{-\infty}^{+\infty} H_k(t, A)\, e^{-\frac{At^2}{2}} f(t)\, dt\right),$$

and the right Fourier series of $f \in L_A^2(\mathbb{R}, \mathbb{C}^{r\times r})$ with respect to $\{H_n(\cdot, A)\}_{n\geqslant 0}$ is defined by

$$S(f)(x) = \sum_{n\geqslant 0} H_n(x, A) C_n(f).$$

With these definitions, a similar version of Theorem 2 for the right case can easily be derived by adapting the previously outlined case.

### 3.2. A numerical application: matrix exponential computation

Let $A$ be a matrix in $\mathbb{C}^{r\times r}$. The problem of computing $e^A$ has attracted considerable attention both, in the past [9] and in recent years [10]. According to Ref. [8], one has

$$e^{xtA-t^2 I} = \sum_{n\geqslant 0} \frac{1}{n!} H_n\left(x, \frac{1}{2}A^2\right) t^n, \quad |t| < \infty. \tag{14}$$

It is important to pay attention to the fact that the matrix $A$ which defines the Hermite matrix polynomial sequence must be *positive definite*, see [3, p. 196], *i.e.* $\mathrm{Re}(z) > 0$ for all $z \in \sigma(A)$. This positive stable condition was imposed on the matrix $A$ to guarantee the existence of $\sqrt{A}$ and some integral properties of Hermite polynomials [8]. Note, however, that this condition is not required for expansion Eq. (14). In an analogous manner to the demonstration of Theorem 1, one finds the following bound:

$$\left\|H_n\left(x, \frac{1}{2}A^2\right)\right\|_2 \leqslant n!\, e^{(|x|\|A\|_2+1)}, \quad \forall\, x \in \mathbb{R},\ n \geqslant 0, \quad \forall\, A \in \mathbb{C}^{r\times r}. \tag{15}$$

Using Eq. (15) in the form

$$\left\|\frac{H_n\left(x, \frac{1}{2}A^2\right)}{n!} t^n\right\|_2 \leqslant |t|^n e^{(|x|\|A\|_2+1)}, \quad n \geqslant 0,$$

and taking into account that $\sum_{n=0}^{\infty}|t|^n$ is convergent for $|t| < 1$, we conclude that convergence of Eq. (14) is uniform for $x$ in any compact interval of $\mathbb{R}$, provided that $|t| < 1$.

Assuming that $x = \lambda$ and $t = \frac{1}{\lambda}$ for $\lambda > 1$, one finds for Eq. (14):

$$e^A = e^{\frac{1}{\lambda^2}} \sum_{n \geqslant 0} \frac{1}{n!\lambda^n} H_n\left(\lambda, \frac{1}{2}A^2\right).$$

Observe that the particular case $\lambda = 1$ is in full agreement with the matrix exponential approximation $E(A; 1; N)$ previously derived in Ref. [3].

We may now define the approximation of the matrix exponential $e^A$ as

$$h_N(\lambda, A) = e^{\frac{1}{\lambda^2}} \sum_{n=0}^{N} \frac{1}{n!\lambda^n} H_n\left(\lambda, \frac{1}{2}A^2\right) \approx e^A. \tag{16}$$

Taking the approximate value $h_N(\lambda, A)$ given by (16) and considering the bound (8), it follows that

$$\begin{aligned} \left\| e^A - h_N(\lambda, A) \right\|_2 &\leqslant e^{\frac{1}{\lambda^2}} \sum_{k \geqslant N+1} \frac{1}{\lambda^k k!} \left\| H_k\left(\lambda, \frac{1}{2}A^2\right) \right\|_2 \\ &\leqslant e^{\frac{1}{\lambda^2}} \sum_{k \geqslant N+1} \frac{e^{\lambda\|A\|_2+1}}{\lambda^k} \\ &= e^{\left(\frac{1}{\lambda^2}+\lambda\|A\|_2+1\right)} \left[ \sum_{k \geqslant 0} \frac{1}{\lambda^k} - \sum_{k=0}^{N} \frac{1}{\lambda^k} \right]. \end{aligned} \tag{17}$$

Simplifying the geometric series in Eq. (17), one finally obtains the error bound for approximation (16):

$$\left\| e^A - h_N(\lambda, A) \right\|_2 \leqslant \frac{e^{\left(\frac{1}{\lambda^2}+\lambda\|A\|_2+1\right)}}{(\lambda - 1)\lambda^N}. \tag{18}$$

For numerical estimates of the bound, let $\varepsilon > 0$ be some fixed *a priori* error. Also, choose $n_0$ to be the first positive integer such that

$$n_0 > \frac{\log\left(\frac{e^{\left(\frac{1}{\lambda^2}+\lambda\|A\|_2+1\right)}}{\varepsilon(\lambda-1)}\right)}{\log\lambda}. \tag{19}$$

The, by combining Eqs. (18) and (19), we conclude

$$\left\| e^A - h_{n_0}(\lambda, A) \right\|_2 \leqslant \varepsilon.$$

In summary, the following result, similar to Theorem 3.1 of Ref. [3], has been proven.

**Theorem 3.** *Let $A$ be a matrix in $\mathbb{C}^{r\times r}$ and let $\lambda > 1$. Let $\varepsilon > 0$. If $n_0$ is the first positive integer such that*

$$n_0 > \frac{\log\left(\frac{e^{\left(\frac{1}{\lambda^2}+\lambda\|A\|_2+1\right)}}{\varepsilon(\lambda-1)}\right)}{\log\lambda}, \tag{20}$$

*then*

$$\left\| e^A - h_{n_0}(\lambda, A) \right\|_2 \leqslant \varepsilon. \tag{21}$$

**Example 1.** For a numerical illustration of Theorem 3 let us consider the following matrix

$$A = \begin{pmatrix} 3 & -1 & 1 \\ 2 & 0 & 1 \\ 1 & -1 & 2 \end{pmatrix}$$

with $\sigma(A) = \{1, 2\}$. Matrix $A$ is non-diagonalizable, and with the help of the minimal theorem the exact value of $\exp(A)$ is shown to be (see Refs. [5, p. 571, 3]):

$$e^A = \begin{pmatrix} 2e^2 & -e^2 & e^2 \\ e(2e-1) & e(1-e) & e^2 \\ e(e-1) & e(1-e) & e^2 \end{pmatrix}.$$

As already pointed out in Ref. [3], for an admissible error of $\varepsilon = 10^{-5}$ we need at least $n_0 = 30$ to provide the required accuracy. Of course, in practice the number of terms to obtain a prefixed accuracy uses to be smaller than the one provided by Theorem 3.1 of Ref. [3], which always supplies a safe estimate. So for instance, taking $n_0 = 19$ and omitting irrelevant digits, one calculates

$$E(A, 1, 19) = \begin{pmatrix} 14.778109507 & -7.389054626 & 7.389054626 \\ 12.059826871 & -4.670771990 & 7.389054626 \\ 4.670772244 & -4.670772244 & 7.389054881 \end{pmatrix},$$

and therefore

$$\left\| e^A - E(A, 1, 19) \right\|_2 = 6.36 \times 10^{-6}.$$

We will compare these results obtained for $\lambda = 1$ in Theorem 3.1 of Ref. [3] with the results from the new Theorem 3.

It is $\|A\|_2 = 4.41302$, which we will use for the evaluation of Eq. (19). It is also convenient to introduce the auxiliary function

$$f(\lambda) := \frac{\log\left( \frac{e^{\left(\frac{1}{\lambda^2} + 4.41302\lambda + 1\right)}}{10^{-5}(\lambda - 1)} \right)}{\log \lambda} \text{ with } \lambda > 1. \tag{22}$$

As Fig. 1 illustrates, this function possesses a minimum in the interval [4, 7]. By using numerical standard routines, we can compute that this minimum is reached at

$$\lambda_0 \approx 4.980662706.$$

Hence, one gets for the minimum

$$f(\lambda_0) \approx 20.6479.$$

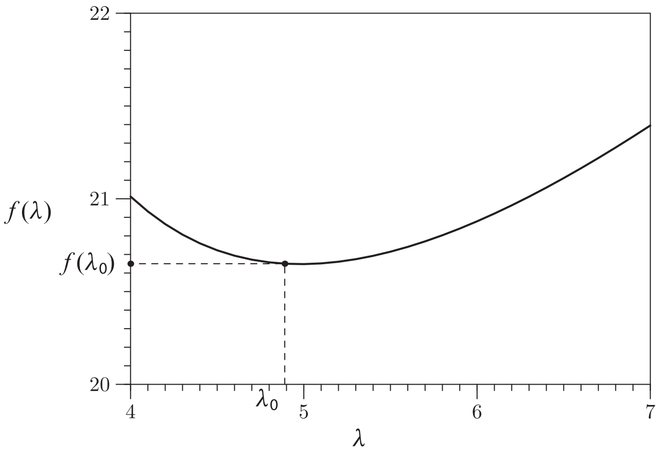


**Fig. 1**. Graph of the function $f(\lambda)$ defined by Eq. (22) with minimum at $\lambda_0 \approx 4.98$ and $\lceil f(\lambda_0)\rceil = 21$.

As a consequence, Theorem 3 with our choice for $\lambda_0$ precisely indicates that we require $n_0 = \lceil f(\lambda_0)\rceil = 21$ approximation steps to reach the prefixed accuracy. In fact, an exact computation yields

$$\left\| e^A - h_{21}(\lambda_0, A)\right\|_2 = 4.626 \times 10^{-15}.$$

Again, it becomes clear that the number of terms required to obtain a prefixed accuracy usually is smaller than the one provided by the more conservative estimate Eq. (21). For instance, taking $n_0 = 12$ yields

$$h_{12}(\lambda_0, A) = \begin{pmatrix} 14.778110374 & -7.389054440 & 7.389054440 \\ 12.059828545 & -4.670772611 & 7.389054440 \\ 4.670774106 & -4.670774106 & 7.389055935 \end{pmatrix},$$

with a corresponding error

$$\left\| e^A - h_{12}(\lambda_0, A)\right\|_2 = 4.212 \times 10^{-6}.$$

## 4. Conclusions

As a continuation and substantial improvement of Ref. [2], this work provides a new upper bound on the 2-norm of the family of Hermite matrix polynomials $H_n(x, A)$, where $A$ is a parameter matrix with all its eigenvalues in the open right-half plane. As indicated in some illustrative examples, this bound is not merely of analytic interest and for use in a general theory of orthogonal matrices, but has potential for several other interesting practical applications.

As a first application a matrix version of the Riemann–Lebesgue lemma for a sequence of Hermite matrix polynomials was introduced. This derivation opens up new avenues to obtain further theorems for matrix function expansions in terms of Hermite matrix polynomials, similar to the analysis already carried out in the existing literature for another class of matrix polynomials [13].

The second application considered an approximation of the matrix exponential as a weighted sum of certain $H_n(x, A)$, to within an error tolerance which may be prescribed *a priori*. The algorithmic steps of the computational process was explained in one specific example.

It is hoped that in future work our proposed matrix expansion for the Hermite case might inspire other interesting applications for matrix calculus.

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