CENTRAL DIAGONAL SECTIONS OF THE n-CUBE

F. A. BARTHA[1], F. FODOR[2], AND B. GONZALEZ MERINO[3]

Abstract. We prove that the volume of central hyperplane sections of a unit cube in $\mathbb{R}^n$ orthogonal to a main diagonal of the cube is a strictly monotonically increasing function of the dimension for $n \geq 3$. Our argument uses an integral formula that goes back to Pólya [Pól13] (see also [Hen79] and [Bal86]) for the volume of central sections of the cube, and Laplace's method to estimate the asymptotic behaviour of the integral. First we show that monotonicity holds starting from some specific n_0. Then, using interval arithmetic (IA) and automatic differentiation (AD), we compute an explicit bound for n_0, and check the remaining cases between 3 and n_0 by direct computation.

1. Introduction

Let $C^n = [-\frac{1}{2}, \frac{1}{2}]^n$ be the unit cube in $\mathbb{R}^n$, and for $u \in \mathbb{R}^n$ let $H(u) = u^\perp$, the hyperplane through o orthogonal to u. We are interested in determining $\mathrm{Vol}_{n-1}(C^n \cap H(u_0))$ in the special case when $u_0 = (1, \ldots, 1) \in \mathbb{R}^n$ is parallel to a main diagonal of C^n.

Hensley [Hen79] described a probabilistic argument, whose origin he attributed to Selberg, proving that $\mathrm{Vol}_{n-1}(C^n \cap H(u_0)) \to \sqrt{6/\pi}$ as $n \to \infty$, and he conjectured that $\max_u \mathrm{Vol}_{n-1}(C^n \cap H(u)) \leq \sqrt{2}$. This conjecture was proved by Ball [Bal86], who proved an integral formula for the volume of sections that goes back to Pólya [Pól13], which, when specialized to the case of $H(u_0)$, is the following:

$$I(n) := \mathrm{Vol}_{n-1}(C^n \cap H(u_0)) = \frac{2\sqrt{n}}{\pi} \int_0^{+\infty} \left(\frac{\sin t}{t}\right)^n dt. \tag{1}$$

It is an interesting fact that the maximum volume hyperplane section of the cube occurs when the hyperplane is orthogonal to $u = (1, 1, 0, \ldots, 0)$, and not for hyperplanes orthogonal to the main diagonals. The limit $\sqrt{6/\pi}$ for the main diagonal is slightly less than $\sqrt{2}$.

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Kerman, Ol'hava and Spektor [KOS15] proved the asymptotic expansion

$$I(n) = \sqrt{\frac{6}{\pi}}\left(1 - \frac{3}{20n} - \frac{13}{1120n^2}\right) + O(n^{-3}), \tag{2}$$

improving the previous computation of Borwein, Borwein and Leonard [BBL10]. However, the size of the error term $O(n^{-3})$ was not computed yet.

It is known that the integral (1) can be evaluated explicitly as

$$\mathrm{Vol}_{n-1}(C^n \cap H(u_0)) = \frac{\sqrt{n}}{2^n(n-1)!}\sum_{i=0}^{n}(-1)^i\binom{n}{i}(n-2i)^{n-1}\mathrm{sign}(n-2i), \tag{3}$$

see Goddard [God45], Grimsey [Gri45], Butler [But60], and Frank and Riede [FR12]. Numerical computations with (3) suggest that $\mathrm{Vol}_{n-1}(C^n \cap H(u_0))$ is a strictly monotonically increasing function of n while it tends to the limit $\sqrt{6/\pi}$ as $n \to \infty$. However, (3) does not seem to lend itself as a tool for proving this monotonicity property.

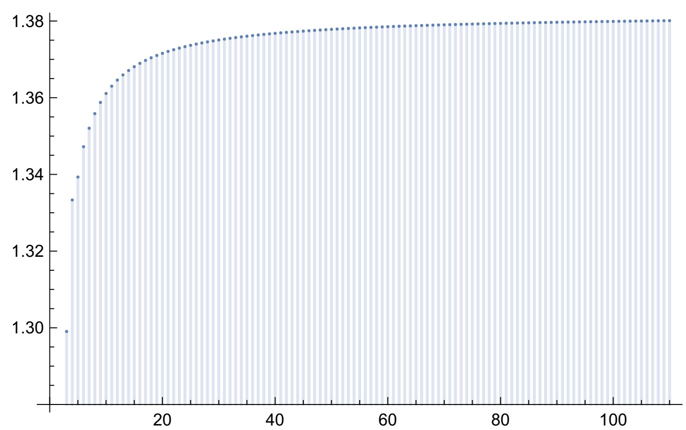

Figure 1. $\mathrm{Vol}_{n-1}(C^n \cap H(u_0))$ for $3 \le n \le 110$ plotted by *Mathematica*.

Recently, König and Koldobsky proved that, in fact, $\mathrm{Vol}_{n-1}(C^n \cap H) \le \sqrt{6/\pi}$ for all $n \ge 2$, see [KK19, Prop. 6(a)]. We also point out the recent result of Aliev [Ali20] (see also [Ali08]) about hyperplane sections of the cube, in which he proves that

$$\frac{\sqrt{n}}{\sqrt{n+1}} \le \frac{I(n+1)}{I(n)} \tag{4}$$

which is slightly less than the monotonicity of $\mathrm{Vol}_{n-1}(C^n \cap H(u_0))$.

For a more detailed overview of the currently known information on sections of the cube and for further references, see, for example, the books of Berger [Ber10] and Zong [Zon06], and the papers by Ball [Bal86, Bal89], König, Koldobsky [KK19] and Ivanov, Tsiutsiurupa [IT20].

Our main result is the following.

Theorem 1. *The volume $Vol_{n-1}(C^n \cap H(u_0))$ is a strictly monotonically increasing function of n for all $n \ge 3$.*

Theorem 1 directly yields the following corollary (which has already been proved by König and Koldobsky [KK19]), and slightly improves the estimate (4) of Aliev mentioned above. It also computes the size of the error term in (2).

Corollary 1. *For any integer $n \geq 2$, it holds that*

$$Vol_{n-1}(C^n \cap H(u_0)) < \sqrt{\frac{6}{\pi}}.$$

and this upper bound is best possible.

The rest of the paper is organized as follows. In Section 2 we use Laplace's method to study the behaviour of the integral (1), and prove the existence of an integer n_0 with the property that $\mathrm{Vol}_{n-1}(C^n \cap H(u_0))$ is an increasing sequence for all $n \geq n_0$. In the Appendix, using interval arithmetic, automatic differentiation, and some analytical arguments, we provide rigorous numerical estimates, which we use in Section 3 to obtain an explicit upper bound on n_0. Finally, we check monotonicity for $3 \leq n \leq n_0$ by calculating the value of of $\mathrm{Vol}_{n-1}(C^n \cap H(u_0))$ using (3), thus concluding the proof of Theorem 1.

2. Proof of the monotonicity for large n

In this section, we prove the following statement which is the most important ingredient of the proof of Theorem 1.

Theorem 2. *There exists an integer n_0 such that $Vol_{n-1}(C^n \cap H(u_0))$ is a strictly monotonically increasing function of n for all $n \geq n_0$.*

Proof. We are going to examine the behaviour of the integral:

$$I(n) = \frac{2\sqrt{n}}{\pi} \int_0^{+\infty} \left(\frac{\sin t}{t}\right)^n dt, \quad n \geq 3.$$

We wish to prove that there exists an n_0 such that $I(n)$ is strictly monotonically increasing for all $n \geq n_0$.

We start the argument by restricting the domain of integration to a finite interval that contains most of the integral as $n \to \infty$. If a fixed, with $1 < a < \pi/2$, then for $n \geq 3$ it holds that

$$\frac{2\sqrt{n}}{\pi} \int_a^{+\infty} \left|\frac{\sin t}{t}\right|^n dt < \frac{2\sqrt{n}}{\pi} \int_a^{+\infty} t^{-n} dt = \frac{2\sqrt{n}}{\pi} \frac{a^{-n+1}}{n-1} < \frac{2}{3} a^{-n} =: e_1(n).$$

Note that the function $e_1(n)$ tends to 0 exponentially fast as $n \to +\infty$. Let a be fixed, say, $a = e^{1/6}$ and define

$$I_a(n) := \frac{2\sqrt{n}}{\pi} \int_0^a \left(\frac{\sin t}{t}\right)^n dt, \quad \text{for } n \geq 3. \tag{5}$$

Then

$$|I(n) - I_a(n)| < e_1(n) \quad \text{for } n \geq 3.$$

We will use Laplace's method to study the behaviour of $I_a(n)$. Let us make the following change of variables

$$\frac{\sin t}{t} = e^{-x^2/6}, \text{ thus } x = \sqrt{-6 \log \frac{\sin t}{t}},$$

where we define the value of $\sin t/t$ to be 1 at $t = 0$. Since $\sin t/t = e^{-t^2/6} + O(t^4)$, the substitution above yields $t \simeq x$ near $t = 0$. Therefore, $x(t)$ is analytic in the interval $[0, a]$. Note that $x(0) = 0$, and $x'(t) > 0$ for all $t \in [0, a]$. Thus, $x(t)$ maps $[0, a]$ bijectively onto $[0, x(a)]$, and so it has an inverse $t(x) : [0, x(a)] \to [0, a]$, which is also analytic in $[0, x(a)]$ by the Lagrange Inversion Theorem because $x'(t) \neq 0$ for $t \in [0, a]$. In our case, $1.211 < x(a) = x(e^{1/6}) = 1.211 \cdots < 1.212$.

The Taylor series of $x(t)$ around $t = 0$ begins with the terms

$$x = t + \frac{t^3}{60} + \frac{139t^5}{151200} + \frac{83t^7}{1296000} + \dots.$$

We can get the first few terms of the Taylor series expansion of $t = t(x)$ around $x = 0$ by inverting the Taylor series of $x(t)$ at $t = 0$ as follows:

$$t(x) = x - \frac{x^3}{60} - \frac{13x^5}{151200} + \frac{x^7}{336000} + \dots.$$

Then

$$t'(x) = 1 - \frac{x^2}{20} - \frac{13x^4}{30240} + R_6(x)$$

is the order 5 Taylor polynomial of $t'(x)$ around $x = 0$ (observe that the degree 5 term is zero), and for the Lagrange remainder term $R_6(x)$, it holds that

$$R_6(x) = \frac{t^{(7)}(\xi)}{6!} x^6$$

for some $\xi \in (0, x)$ (depending on x). Since $t(x)$ is analytic in $[0, x(a)]$, in particular the seventh derivative of $t(x)$ is analytic too, and thus it is a continuous function. Then the Extreme Value Theorem yields that $t^{(7)}$ attains its maximum in $[0, x(a)]$, and thus $|t^{(7)}(x)| \leq R$, for some $R > 0$ and every $x \in [0, x(a)]$. Then we can use the following estimate on $x \in [0, x(a)]$:

$$|R_6(x)| \leq \frac{R}{6!} x^6, \tag{6}$$

Therefore, after the change of variables, we need to evaluate

$$\begin{aligned} I_a(n) &= \frac{2\sqrt{n}}{\pi} \int_0^{x(a)} e^{-nx^2/6} t'(x) dx \\ &= \frac{2\sqrt{n}}{\pi} \int_0^{x(a)} e^{-nx^2/6} \left(1 - \frac{x^2}{20} - \frac{13x^4}{30240} + R_6(x)\right) dx \\ &= \frac{2\sqrt{n}}{\pi} \int_0^{x(a)} e^{-nx^2/6} \left(1 - \frac{x^2}{20} - \frac{13x^4}{30240}\right) dx \\ &+ \frac{2\sqrt{n}}{\pi} \int_0^{x(a)} e^{-nx^2/6} R_6(x) dx. \end{aligned} \tag{7}$$

In order to calculate the above integrals we will use the central moments of the normal distribution: If $y = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$, then for an integer $p \geq 0$ it holds that

$$\mathbb{E}[y^p] = \begin{cases} 0, & \text{if } p \text{ is odd}, \\ \sigma^p (p-1)!!, & \text{if } p \text{ is even}. \end{cases} \tag{8}$$

In our case $\sigma^2 = 3/n$ and $p = 6$. Thus, using (8) and (6), we get that

$$\begin{aligned} \frac{2\sqrt{n}}{\pi}\int_0^{x(a)} e^{-nx^2/6}|R_6(x)|dx &\le \frac{2R\sqrt{n}}{\pi 6!}\int_0^{x(a)} e^{-nx^2/6}x^6 dx \\ &< \frac{2R\sqrt{n}}{\pi 6!}\int_0^{+\infty} e^{-nx^2/6}x^6 dx \\ &= \frac{2R\sqrt{n}}{\pi 6!}\frac{3^3}{n^3}5!! \\ &= \frac{9R}{8\pi}\frac{1}{n^{5/2}} \\ &< \frac{R}{2}\frac{1}{n^{5/2}} =: e_2(n). \end{aligned} \tag{9}$$

Notice also that

$$\begin{aligned} &\frac{2\sqrt{n}}{\pi}\int_0^{+\infty} e^{-nx^2/6}\left(1 - \frac{x^2}{20} - \frac{13x^4}{30240}\right)dx \\ &= \sqrt{\frac{3\pi}{2}}\frac{2\sqrt{n}}{\pi}\left(\frac{1}{n^{1/2}} - \frac{3}{20n^{3/2}} - \frac{13}{1120n^{5/2}}\right) \\ &= \sqrt{\frac{6}{\pi}}\left(1 - \frac{3}{20n} - \frac{13}{1120n^2}\right). \end{aligned} \tag{10}$$

The complementary error function is defined as

$$\operatorname{erfc}(x) := 2\frac{1}{\sqrt{\pi}}\int_x^{+\infty} e^{-\tau^2}d\tau.$$

It is known that $\operatorname{erfc}(x) \le e^{-x^2}$ for $x \ge 0$. Then, taking into account that $x(a) > 1.211$, we obtain

$$\begin{aligned} &\frac{2\sqrt{n}}{\pi}\left|\int_{x(a)}^{+\infty} e^{-nx^2/6}\left(1 - \frac{x^2}{20} - \frac{13x^4}{30240}\right)dx\right| \\ &\le \frac{2\sqrt{n}}{\pi}\int_{x(a)}^{+\infty} e^{-nx^2/6}\left|1 - \frac{x^2}{20} - \frac{13x^4}{30240}\right|dx \\ &\le \frac{2\sqrt{n}}{\pi}\int_{x(a)}^{+\infty} e^{-nx^2/6}\left(1 + \frac{x^2}{20} + \frac{13x^4}{30240}\right)dx \\ &< \frac{2\sqrt{n}}{\pi}\int_1^{+\infty} e^{-nx^2/6}\left(1 + \frac{x^2}{20} + \frac{13x^4}{30240}\right)dx \\ &= \sqrt{\frac{6}{\pi}}\operatorname{erfc}(\sqrt{n/6})\left(\frac{13 + 168n + 1120n^2}{1120n^2}\right) + 2e^{-n/6}\sqrt{n}\frac{117 + 1525n}{10080\pi n^2} \\ &< \frac{5}{3}e^{-n/6} =: e_3(n). \end{aligned} \tag{11}$$

Now, using the monotonicity of $e_1(n)$, we obtain that

$$I(n+1) - I(n) \ge (I_a(n+1) - e_1(n+1)) - (I_a(n) + e_1(n)) \ge I_a(n+1) - I_a(n) - 2e_1(n).$$

Furthermore, expressing I_a (cf. (7)) as a difference of integrals in the intervals $[0, +\infty)$ and $[x(a), +\infty)$, together with the value of the integral in $[0, +\infty)$ (10) and the bounds (9) and (11), yields

$$I_a(n+1) \geq \sqrt{\frac{6}{\pi}}\left(1 - \frac{3}{20(n+1)} - \frac{13}{1120(n+1)^2}\right) - e_2(n+1) - e_3(n+1),$$

and

$$I_a(n) \leq \sqrt{\frac{6}{\pi}}\left(1 - \frac{3}{20n} - \frac{13}{1120n^2}\right) + e_2(n) + e_3(n).$$

Therefore

$$\begin{aligned}
I(n+1) - I(n) &\geq \sqrt{\frac{6}{\pi}}\left(\frac{3}{20n} - \frac{3}{20(n+1)} + \frac{13}{1120n^2} - \frac{13}{1120(n+1)^2}\right) \\
&\quad - 2e_1(n) - e_2(n) - e_2(n+1) - e_3(n) - e_3(n+1) \\
&> \sqrt{\frac{6}{\pi}}\left(\frac{3}{20n(n+1)} + \frac{13(2n+1)}{1120n^2(n+1)^2}\right) \\
&\quad - \frac{4}{3}a^{-n} - (e_2(n) + e_2(n+1) + e_3(n) + e_3(n+1)) \\
&> \sqrt{\frac{6}{\pi}}\left(\frac{3}{20n(n+1)}\right) - \frac{4}{3}a^{-n} - 2e_2(n) - 2e_3(n) \\
&> \sqrt{\frac{6}{\pi}}\left(\frac{3}{20n(n+1)}\right) - \frac{4}{3}a^{-n} - \frac{R}{n^{5/2}} - \frac{10}{3}e^{-n/6} \\
&= \sqrt{\frac{6}{\pi}}\left(\frac{3}{20n(n+1)}\right) - \frac{14}{3}e^{-n/6} - \frac{R}{n^{5/2}}. \qquad (12)
\end{aligned}$$

Clearly, there exists an n_0, such that for all $n \geq n_0$ the expression (12) is strictly positive. Therefore, $\mathrm{Vol}_{n-1}(C^n \cap H(u_0))$ is strictly monotonically increasing for $n \geq n_0$.

Thus, we have finished the proof of Theorem 2. □

Remark. Figure 1 suggests that $\mathrm{Vol}_{n-1}(C_n \cap H(u_0))$ is not only a monotonically increasing sequence but also concave, i.e., $2I(n+1) \geq I(n) + I(n+2)$ for $n \geq 4$. We note, without giving the details, that with a similar argument as in the proof of Theorem 2, but using more terms of the Taylor expansion of $t(x)$, one can also show that

$$\begin{aligned}
&2I(n+1) - I(n) - I(n+2) \\
&\quad \geq 2I_a(n+1) - I_a(n) - I_a(n+2) - \xi_1 e_1(n) - \xi_2 e_2(n) - \xi_3 e_3(n) \\
&\quad \geq \frac{3\sqrt{3}}{5\sqrt{2\pi}} \frac{1}{n(n+1)(n+2)} + O(n^{-4}) - \xi_1 e_1(n) - \xi_2 e_2(n) - \xi_3 e_3(n),
\end{aligned}$$

for some $\xi_i > 0$, $i = 1, 2, 3$. If we take into account sufficiently many terms of the Taylor series of $t(x)$, then we can guarantee that each error term is of smaller order than n^{-3}, and thus there exists a number n_1 such that the sequence $I(n)$ is concave for all $n \geq n_1$.

3. Proof of Theorem 1

In order to prove Theorem 1, we need an explicit upper bound on the critical number n_0. Using a combination of interval arithmetic, automatic differentiation, and some analytic methods, we can obtain a rigorous upper estimate for the seventh derivative $|t^{(7)}(x)|$ in $x \in [0, x(a)]$. We provide the details of this argument in the Appendix. Here, we only quote the following upper bound (see Theorem 3 part (3)):

$$R \leq 0.79461. \tag{13}$$

Now, substituting the estimate (13) in inequality (12), we get that $n_0 = 75$. Then, we can calculate the values of $I(n+1) - I(n)$ using (3) to the required accuracy, and verify monotonicity for all $3 \leq n \leq 75$, see Figure 2 below.

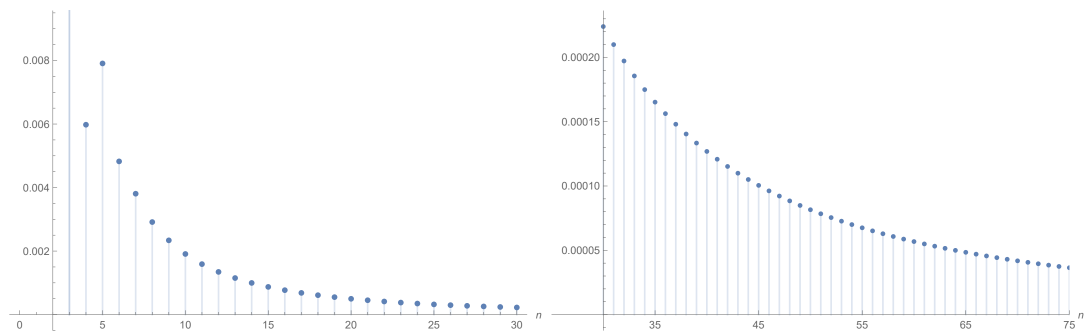

FIGURE 2. $I(n+1) - I(n)$ for $3 \leq n \leq 75$ plotted by *Mathematica*

Remark. Using the same ideas as above, one could show the concavity of $I(n)$ for $n \geq 3$.

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Appendix

Consider the function

$$x(t) = \sqrt{-6\log\left(\frac{\sin t}{t}\right)}, \tag{14}$$

where $t \in [0, 1.2]$. The fraction $\frac{\sin t}{t}$ is understood to be augmented with its limit at $t = 0$ that is $\frac{\sin 0}{0} = 1$. Then, the function $x(t)$ is analytic.

Theorem 3. *The following holds true.*

(1) $x(t)$ *is strictly increasing on* $[0, 1.2]$ *and*

$$x(t) \leq 1.231399 \qquad \text{for } t \in [0, 1.2].$$

(2) $x(t)$ *is invertible with inverse* $t(x)$*, where* $x \in [0, x(1.2)]$.

(3) *The 7th derivative of* $t(x)$ *attains the upper bound*

$$\left|t^{(7)}(x)\right| \leq 0.79461 \qquad \text{for } x \in [0, x(1.2)].$$

The monotonicity stated in (1) is trivial, hence, one just needs to establish the containment $x(1.2) \in [0, x(1.2)]$. Note that (2) is a consequence of (1), thus, in the following we will deal with evaluating $x(t)$ and proving (3).

There are numerous computational steps involved. In order to obtain rigorous results, we have based our computations on two techniques, namely, *interval arithmetic (IA)* and *automatic differentiation (AD)* that are capable of providing mathematically sound bounds for functions and their derivatives alike. Besides the technical hurdle, severe difficulties arise at the left endpoint $t = 0$ as, when computing the derivatives of $x(t)$, we need to differentiate both $\sqrt{\cdot}$ and $\frac{\sin t}{t}$ at zero. It was tempting to use Taylor models, an advanced combination of these two, however that could still not handle the aforementioned left endpoint directly, hence, we chose to stick with the straightforward application of the two techniques and used the CAPD package [CG20]. For a comprehensive overview of these topics we refer to [Tuc, Gri, Mak03].

We emphasize that the major goal of Theorem 3 is providing the given bounds, hence, we made little effort to obtain tighter results and were performing sub–optimal computations knowingly, in order to decrease the implementation burden.

The key step to overcome the difficulties at $t = 0$ is to rephrase (14) as

$$\begin{aligned} x(t) &= t\sqrt{h(t)}, \\ h(t) &= (g \circ F_2)(t) \cdot (-6F(t)), \\ g(t) &= \frac{\log(1+t)}{t}, \\ F_2(t) &= t^2 F(t), \qquad\qquad \text{and} \\ F(t) &= \frac{\frac{\sin(t)}{t} - 1}{t^2}. \end{aligned} \tag{15}$$

Section 5 details the considerations used for dealing with the functions appearing in (15). In particular, Sections 5.1 and 5.2 handle the functions $\frac{\sin t}{t}$ and $F(t)$; a computational scheme for their derivatives is provided. Then, we turn our attention to $\frac{\log(1+t)}{t}$ and derive analogous results in Section 5.3. The square root is discussed in Section 5.4. Then, in Section 5.5, we present a pure formula for the higher order chain–rule used to compose $g(t)$ and $F_2(t)$. Section 6 contains the results for $x(t)$ and its derivatives, in particular, the proof of the remaining part of (1) in Theorem 3. Section 7 deals with $t(x)$ by giving a general inversion procedure in Section 7.1 and the final proof in Section 7.2.

The codes performing the rigorous computational procedure described in this manuscript, together with the produced outputs, are publicly available at [FAB20].

5. Bounding functions and their derivatives

First, we will closely analyze some Taylor expansions centered at $t_0 = 0$ and derive bounds for Taylor coefficients of the very same functions expanded around another center point $\hat{t_0}$. Then, we include the higher order chain–rule for completeness.

5.1. The function $\frac{\sin t}{t}$.

The Taylor series of $\sin t$ centered at $t_0 = 0$ is given as

$$\sin t = \sum_{k=0}^{\infty} (-1)^k \frac{t^{2k+1}}{(2k+1)!}$$

and is convergent for all $t \in \mathbb{R}$. Consequently, we obtain the Taylor series of

$$f(t) := \begin{cases} \frac{\sin t}{t}, & \text{if } t > 0, \\ 1, & \text{if } t = 0 \end{cases}$$

as

$$f(t) = \sum_{k=0}^{\infty} (-1)^k \frac{t^{2k}}{(2k+1)!}, \tag{16}$$

again, centered at $t_0 = 0$ with the same convergence radius. Therefore,

$$\frac{1}{m!} f^{(m)}(t) = \frac{1}{m!} \sum_{k \geq m/2}^{\infty} (-1)^k \frac{t^{2k-m}}{(2k-m)! \cdot (2k+1)} \qquad \text{for } m = 0, 1, \ldots \tag{17}$$

We shall bound these infinite series as follows. Let $N \geq m/2$, then, define the finite part $S_f(t; N, m)$ and the remainder part $E_f(t; N, m)$ as

$$
\begin{aligned}
S_f(t; N, m) &= \frac{1}{m!} \sum_{k \geq m/2}^{N} (-1)^k \frac{t^{2k-m}}{(2k-m)! \cdot (2k+1)} \qquad \text{and} \\
E_f(t; N, m) &= \frac{1}{m!} \sum_{k=N+1}^{\infty} (-1)^k \frac{t^{2k-m}}{(2k-m)! \cdot (2k+1)}.
\end{aligned} \tag{18}
$$

The following lemma establishes bounds for the remainder.

Lemma 1. *Let $m, N \in \mathbb{Z}$ with $m \geq 0$ and $N \geq m/2$. Then,*

$$E_f(t; N, m) \in \frac{1}{m!} \frac{e^{\,t}}{(2N+2-m)!} t^{2N+2-m} \ \cdot \ [-1, 1]$$

for all $t \geq 0$.

Proof. Let $t \geq 0$ and consider

$$|E_f(t; N, m)| \leq \frac{1}{m!} \sum_{k=N+1}^{\infty} \frac{t^{2k-m}}{(2k-m)! \cdot (2k+1)} \leq \frac{1}{m!} \sum_{k=N+1}^{\infty} \frac{t^{2k-m}}{(2k-m)!} \leq \frac{1}{m!} \sum_{k=2N+2-m}^{\infty} \frac{t^k}{k!}.$$

Note that we have obtained the tail of the Taylor series of the exponential function centered at $t_0 = 0$. The corresponding Lagrange remainder gives us that for all integers $K \geq 0$

$$\sum_{k=K}^{\infty} \frac{t^k}{k!} = \frac{1}{K!} \frac{\mathrm{d}^K e^t}{\mathrm{d}t^K}(\xi) \cdot t^K$$

holds with some $\xi = \xi(K) \in [0, t]$. Observe that $\frac{\mathrm{d}^K e^t}{\mathrm{d}t^K}(\xi) = e^{\xi}$ and that attains its maximum at $\xi = t$ over $\xi \in [0, t]$. Hence, we obtain

$$\sum_{k=K}^{\infty} \frac{t^k}{k!} \leq \frac{1}{K!} e^{\,t} \cdot t^K \qquad \text{for } t \geq 0.$$

Finally, setting $K = 2N + 2 - m$ and deriving a bound on $E_f(t; N, m)$ from the estimate for $|E_f(t; N, m)|$ concludes the proof. □

Defining

$$\mathbf{E}_f(t; N, m) = \frac{1}{m!} \frac{e^{\,t}}{(2N+2-m)!} t^{2N+2-m} \ \cdot \ [-1, 1] \tag{19}$$

together with (17), (18), and Lemma 1 gives a rigorous computational scheme for $f(t)$ and its derivatives, namely,

$$\frac{1}{m!} f^{(m)}(t) \in S_f(t; N, m) + \mathbf{E}_f(t; N, m).$$

We remark that $\lim_{N \to \infty} \mathbf{E}_f(t; N, m) \to \{0\}$ for all $t \in \mathbb{R}$ and $m \geq 0$. Figure 3 gives an insight on how the obtained bound for the remainder behaves.

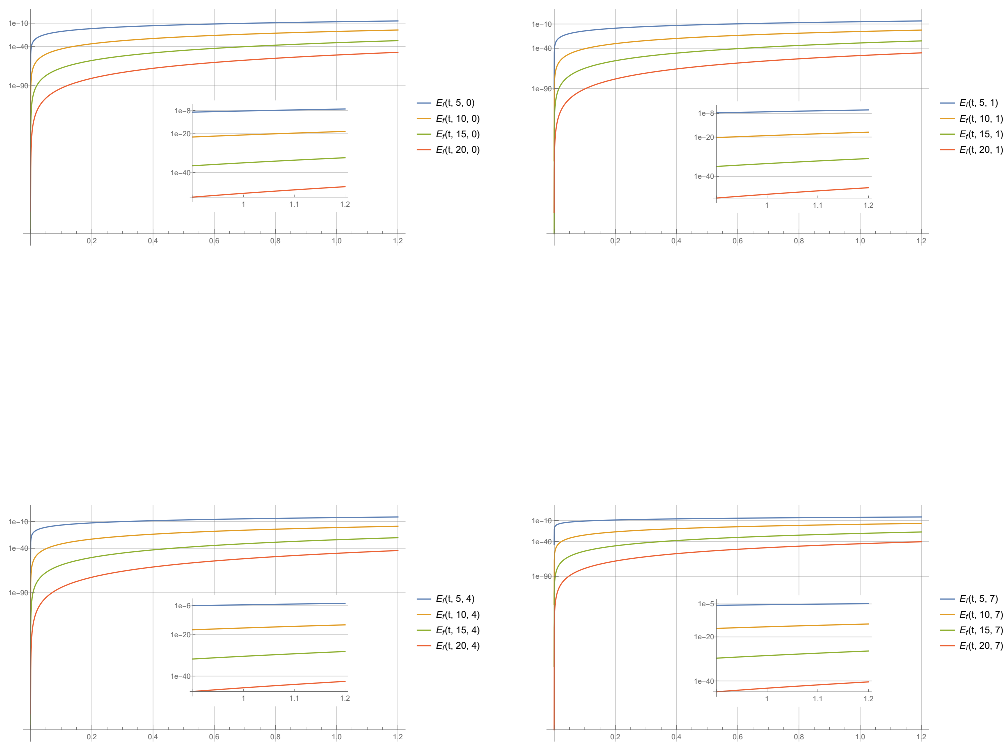

FIGURE 3. The upper bound of $\mathbf{E}_f(t; N, m)$ for various (N, m) over $t \in [0, 1.2]$.

5.2. **The function** $1 + t^2 F(t) = \frac{\sin t}{t}$**.** Even though there are no issues with directly computing $\log(f(t))$ using the results above, as shown in (15), we will need a more sophisticated approach in order to be able to tackle the final square root operation in the neighbourhood of zero. To that end, we rewrite expansion (16) as

$$f(t) = 1 + t^2 F(t) = 1 + t^2 \sum_{k=0}^{\infty} (-1)^{k+1} \frac{t^{2k}}{(2k+3)!},$$

a 2nd–order Taylor model. Analogous arguments, as in Section 5.1, lead to the following.

Lemma 2.

$$\frac{1}{m!} F^{(m)}(t) \in S_F(t; N, m) + \mathbf{E}_F(t; N, m),$$

where

$$S_F(t;N,m) = \frac{1}{m!}\sum_{k\geq m/2}^{N}(-1)^{k+1}\frac{t^{2k-m}}{(2k-m)!\cdot(2k+1)(2k+2)(2k+3)} \qquad \textit{and}$$
$$\mathbf{E}_F(t;N,m) = \mathbf{E}_f(t;N,m).$$

Note that the remainder bound is identical to the one in (19) as the factor in the denominator $(2k+1)(2k+2)(2k+3)$ may be eliminated the same way as $(2k+1)$ in the proof of Lemma 1.

5.3. **The function $\frac{\log(1+t)}{t}$.** Following (15), we will compute $x(t)$ using the form

$$x(t) = t\sqrt{-6\,F(t)\frac{\log\left(1+t^2F(t)\right)}{t^2F(t)}}.$$

Thus, the next step is to analyze $g(t) = \frac{\log(1+t)}{t}$, where $t \in (-1,1)$. This interval comes from the well-known expansion of $\log(1+t)$. At $t=0$, we augment with the limit $g(0) := 1$. Note that the argument of $g(\cdot)$ will be $t^2F(t) = \frac{\sin t}{t} - 1$ that takes values roughly in $[-0.223, 0]$.

Let us start from the Taylor series of $\log(1+t)$ centered at $t_0 = 0$, namely,

$$\log(1+t) = \sum_{k=1}^{\infty}(-1)^{k+1}\frac{t^k}{k}$$

that is convergent for $|t| < 1$. Then, formally,

$$g(t) = \sum_{k=0}^{\infty}(-1)^k\frac{t^k}{k+1}$$

and

$$\frac{1}{m!}g^{(m)}(t) = \frac{1}{m!}(-1)^m\sum_{k=0}^{\infty}(-1)^k\frac{t^k}{k+m+1}\,\frac{(k+m)!}{k!} \qquad \text{for } m = 0,1,\ldots$$

that can be simplified as

$$\frac{1}{m!}g^{(m)}(t) = (-1)^m\sum_{k=0}^{\infty}(-1)^k\binom{k+m}{m}\frac{t^k}{k+m+1}.$$

We define

$$\begin{aligned} S_g(t;N,m) &= (-1)^m\sum_{k=0}^{N}(-1)^k\binom{k+m}{m}\frac{t^k}{k+m+1} \qquad \text{and} \\ E_g(t;N,m) &= (-1)^m\sum_{k=N+1}^{\infty}(-1)^k\binom{k+m}{m}\frac{t^k}{k+m+1} \end{aligned} \tag{20}$$

for $N \geq 0$ (practically $N \geq m$ so that $k+m > 2m$ in the binomial coefficients in E_g). We may bound the remainder part as detailed below.

Lemma 3. *Let $N \geq m \geq 0$ and $t \in (-1,1)$. Then,*

$$|E_g(t;N,m)| \leq \begin{cases} \frac{|t|^{N+1}}{(1-|t|)^{N+2}}, & \textit{if } m = 0, \\ \left(\frac{2e}{m}\right)^m m!\binom{m+N+1}{m}\frac{|t|^{N+1}}{(1-|t|)^{m+N+2}}, & \textit{else.} \end{cases}$$

Proof. When $m = 0$, the binomial coefficient $\binom{k+m}{m} = 1$, thus,

$$|E_g(t; N, 0)| \leq \sum_{k=N+1}^{\infty} \frac{|t|^k}{k+1} \leq \sum_{k=N+1}^{\infty} |t|^k.$$

On the other hand, for $m > 0$, it is known that

$$\binom{k+m}{m} \leq \left(\frac{e\,(k+m)}{m}\right)^m .$$

Hence,

$$|E_g(t; N, m)| \leq \sum_{k=N+1}^{\infty} \left(\frac{e\,(k+m)}{m}\right)^m \frac{|t|^k}{k+m+1} \leq$$
$$\sum_{k=N+1}^{\infty} \left(\frac{e\,(1+\frac{m}{k})}{m}\right)^m \frac{k^m |t|^k}{k+m+1} \leq \left(\frac{2e}{m}\right)^m \sum_{k=N+1}^{\infty} k^m |t|^k.$$

Thus, for both cases, it is sufficient to bound the series

$$\sum_{k=N+1}^{\infty} k^m |t|^k$$

for all $m = 0, 1, \dots\,, N \geq m$ and $|t| < 1$.

In order to simplify the notation, let $T = |t| \in [0, 1)$ and consider the m-th derivative of the convergent geometric series

$$\frac{1}{1-T} = \sum_{k=0}^{\infty} T^k$$

that is

$$\left(\frac{1}{1-T}\right)^{(m)} = \sum_{k=0}^{\infty} \frac{(k+m)!}{k!} T^k.$$

We may easily bound the remainder of this series starting from $k = N+1$ using, again, the Lagrange formula as

$$\sum_{k=N+1}^{\infty} \frac{(k+m)!}{k!} T^k = \frac{\mathrm{d}^{m+N+1}}{\mathrm{d}T^{m+N+1}} \frac{1}{1-T}\bigg|_{T=\xi} \cdot \frac{1}{(N+1)!} \cdot T^{N+1}$$

with some $\xi \in [0, T]$. The K-th derivative of $\frac{1}{1-T} = (1-T)^{-1}$ is given by $K!\,(1-T)^{-(K+1)}$ that is clearly maximal for $\xi = T$. Hence,

$$\sum_{k=N+1}^{\infty} \frac{(k+m)!}{k!} T^k \leq (m+N+1)!\,(1-T)^{-(m+N+2)} \frac{1}{(N+1)!} T^{N+1}$$

that concludes the proof by noting that

$$\sum_{k=N+1}^{\infty} k^m T^k \leq \sum_{k=N+1}^{\infty} \frac{(k+m)!}{k!} T^k$$

holds for all $N \geq m \geq 0$ and $T \in [0, 1)$. □

In summary, letting

$$\mathbf{E}_g(t; N, m) := [-1, 1] \cdot \begin{cases} \frac{|t|^{N+1}}{(1-|t|)^{N+2}}, & \text{if } m = 0, \\ \left(\frac{2e}{m}\right)^m m! \binom{m+N+1}{m} \frac{|t|^{N+1}}{(1-|t|)^{m+N+2}}, & \text{else,} \end{cases}$$

provides the computational method

$$\frac{1}{m!} g^{(m)}(t) \in S_g(t; N, m) + \mathbf{E}_g(t; N, m). \tag{21}$$

To analyze the dynamics of (21), observe that the behaviour of the remainder is governed by

$$\binom{m+N+1}{m} \left(\frac{|t|}{1-|t|}\right)^N$$

for fixed $t \in (-1, 1)$ and $m \geq 0$. Using the same bound as above for the binomial, it is easy to see that, eventually,

$$N^m \left(\frac{|t|}{1-|t|}\right)^N$$

determines the limit, when $N \to \infty$. Therefore,

$$\lim_{N \to \infty} \mathbf{E}_g(t; N, m) = \{0\},$$

when $\frac{|t|}{1-|t|} < 1$ that is $|t| < \frac{1}{2}$. Recall that for our case this will be satisfied as $\frac{\sin 1.2}{1.2} - 1 \approx -0.223$. The dynamics of the upper bound of $\mathbf{E}_g(t; N, m)$ is demonstrated on Figure 4.

5.4. **The function $\sqrt{t^2 h(t)}$.** Assume $t \in [0, T]$ with some $T \geq 0$. By itself, the function $\sqrt{t}$ is not differentiable at $t_0 = 0$. However, if the argument is of the special form $t^2 h(t)$ with $h(t) \neq 0$, then the situation changes as

$$\sqrt{t^2 h(t)} = t\sqrt{h(t)},$$

hence,

$$\frac{\mathrm{d}}{\mathrm{d}t}\sqrt{t^2 h(t)} = \sqrt{h(t)} + t\frac{h'(t)}{2\sqrt{h(t)}}$$

implying no difficulties for all $t \in [0, T]$.

5.5. **The chain–rule.** There are numerous known formulae for the higher order chain rule [Joh02]. We shall use the classical one named after Faà di Bruno that is written as follows.

Lemma 4 (Faà di Bruno). *Let $f\colon I \to U$ and $g\colon U \to V$ be analytic functions, where $I, U, V \subseteq R$ are connected subsets. Consider the Taylor expansions $f(t) = \sum_{k=0}^{\infty} (f)_k (t - t_0)^k$ centered at $t_0 \in I$ with $t \in I$ and $g(x) = \sum_{k=0}^{\infty} (g)_k (x - x_0)^k$ centered at $x_0 = f(t_0)$ for $x \in U$. Then, the composite function $(g \circ f)$ attains the Taylor expansion $(g \circ f)(t) = \sum_{k=0}^{\infty} (g \circ f)_k (t - t_0)^k$ centered at t_0 with the coefficients*

$$(g \circ f)_0 = (g)_0 \qquad \text{and}$$

$$(g \circ f)_k = \sum_{\substack{b_1 + 2b_2 + \ldots + kb_k = k \\ m := b_1 + b_2 + \ldots + b_k}} \frac{m!}{b_1! b_2! \ldots b_k!} (g)_m \prod_{i=1}^{k} \Big((f)_i \Big)^{b_i}, \tag{22}$$

where $k \geq 1$ and $b_1, \ldots, b_k$ are nonnegative integers.

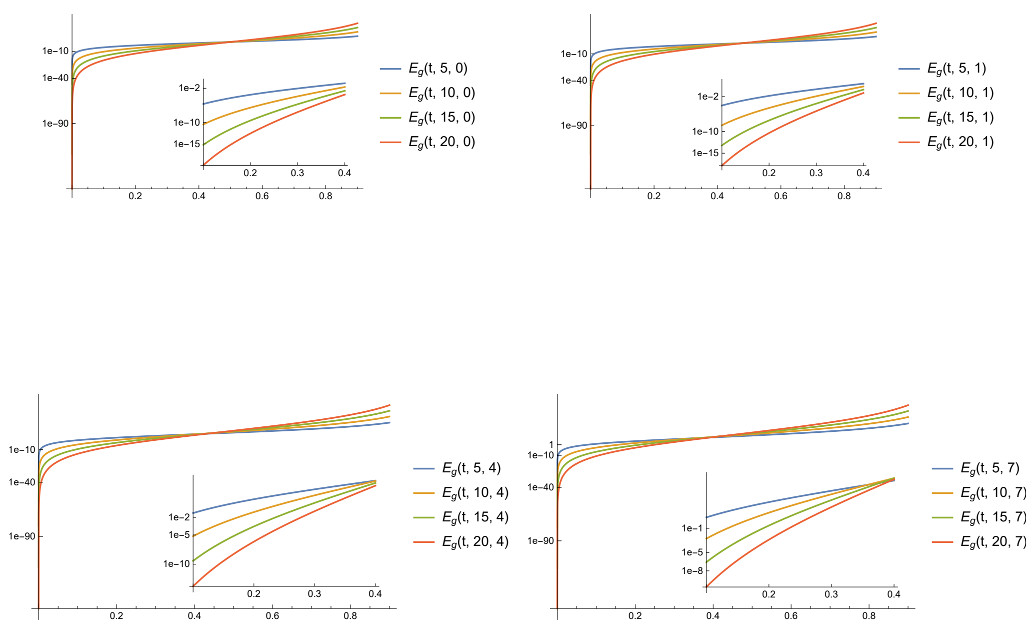

FIGURE 4. The upper bound of $\mathbf{E}_g(t; N, m)$ for various values.

Note that we altered the notation somewhat compared to [Joh02] and use Taylor coefficients instead of derivatives, this should not cause confusion.

6. Derivatives of $x(t)$

Using the combination of results of Section 5, we may attempt to evaluate $x(t)$ and its derivatives based on the steps detailed in (15). The expansions of -6, t, and t^2 are trivial, so is the application of the product rule; for the square root, the computation of Taylor coefficients is straightforward [Tuc, Gri].

We used a uniform $N = 20$ when executing our program and imposed $0 \notin x^{(1)}([0, 1.2])$ to hold as an additional requirement needed for the inverse computations (that was never violated). We have subdivided the original $[0, 1.2]$ into smaller intervals so that each was no longer than ≈ 0.001. For each of these intervals we attempted to compute the expansion of $x(t)$ directly from (14) as well. This clearly failed for those close to $t = 0$, however, whenever it succeeded, we compared it with the results from scheme (15) and used the intersection of the two, somewhat independent, results.

The obtained enclosures are given in Table 1. Each row presents the interval hull of the rigorous bounds obtained over all small subintervals. In particular, the first one establishes the remaining part of (1) in Theorem 3.

Taylor coefficient	**for any $t_0 \in [0, 1.2]$ is contained in**
$(x)_0$	$[0, 1.231398839636382]$
$(x)_1$	$[0.9999999685287251, 1.083235943182105]$
$(x)_2$	$[-2.929687759839051\mathrm{e}{-05}, 0.0801755504333559]$
$(x)_3$	$[0.01666660338755699, 0.03629193622156669]$
$(x)_4$	$[-1.057942939789218\mathrm{e}{-05}, 0.01168468536998257]$
$(x)_5$	$[0.0009192620048196485, 0.005043087325702847]$
$(x)_6$	$[-2.60552431006164\mathrm{e}{-06}, 0.002097914891978437]$
$(x)_7$	$[6.400904923767153\mathrm{e}{-05}, 0.0009395299698464796]$

TABLE 1. **Bounds on Taylor coefficients of $x(t)$ centered at $t_0 \in [0, 1.2]$.**

7. DERIVATIVES OF $t(x)$

Now, that we have computed rigorous bounds for the Taylor coefficients of $x(t)$ up to the desired order for any center $t_0 \in [0, 1.2]$, we turn our attention to its inverse $t(x)$. First, in Section 7.1, we present the general formula for computing the inverse expansion, then, we include the results of our computation for $t(x)$ in Section 7.2, thereby concluding the proof of (3) in Theorem 3.

7.1. **Derivatives of the inverse function.** Practical formulae for Taylor expansion of the inverse function based on the coefficients of the original one are rather scarce. For our purposes it is reasonable to utilize the result of Faà di Bruno, seen in Section 5.5, directly.

Assume that $x(t)$ has the expansion $x(t) = \sum_{k=0}^{\infty} (x)_k\, (t-t_0)^k$ centered at t_0 and $(x)_1 \neq 0$. Then, for the inverse we may construct the expansion $t(x) = \sum_{k=0}^{\infty} (t)_k\, (x - x_0)^k$ centered at $x_0 = x(t_0)$ as

$$
\begin{aligned}
&(t)_0 = t_0, \\
&(t)_1 = \frac{1}{(x)_1}, \qquad \text{and} \\
&(t)_k = -\sum_{\substack{b_1+2b_2+\ldots+kb_k=k \\ m:=b_1+b_2+\ldots+b_k \\ m\neq k}} \frac{m!}{b_1!b_2!\ldots b_k!}\,(t)_m \left((x)_1 \right)^{b_1-k} \prod_{i=2}^{k} \left((x)_i \right)^{b_i},
\end{aligned}
\tag{23}
$$

for $k \geq 2$. The first two coefficients are trivial. The general part is a consequence of Lemma 4 applied to $(t \circ x)(t)$ by observing that $(t \circ x)_k = 0$ for $k \geq 2$ and that in the sum the only term containing $(t)_k$ (that is $(g)_k$ in the original Lemma) is given by $b_1 = k$ and $b_i = 0$ for all other i-s as

$$
\frac{k!}{k!\,1!\ldots 1!}\,(t)_k \left((x)_1 \right)^k = (t)_k \left((x)_1 \right)^k .
$$

7.2. **Proof of (3) in Theorem 3.** We have applied (23) on each of the subintervals and the corresponding expansion of $x(t)$, see Section 6. The interval hull of the results is presented in Table 2. Using that $(t)_7 = \frac{1}{7!} t^{(7)}(x_0)$, we directly obtain the claim of (3) in Theorem 3.

Taylor coefficient	**for any $x_0 \in [0, x(1.2)]$ is contained in**
$(t)_0$	$[0, 1.2]$
$(t)_1$	$[0.9231599138618016, 1.000000031471276]$
$(t)_2$	$[-0.06314379930614004, 2.929687986150493ee{-}05]$
$(t)_3$	$[-0.01786259055874003, -0.01666548440509875]$
$(t)_4$	$[-0.0004384654419668558, 1.546225158582501\text{e}{-}05]$
$(t)_5$	$[-8.966033591264478\text{e}{-}05, 0.0002158420158508729]$
$(t)_6$	$[-8.817887028973888\text{e}{-}05, 0.0001975306217048509]$
$(t)_7$	$[-0.0001247685609928281, 0.0001576597861306056]$

TABLE 2. **Bounds on Taylor coefficients of $t(x)$ centered at $x_0 \in [0, x(1.2)]$.**

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