Numerical Study of the Rate of Convergence of Chernoff Approximations to Solutions of the Heat Equation

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Abstract. Chernoff approximations are a flexible and powerful tool of functional analysis, which can be used, in particular, to find numerically approximate solutions of some differential equations with variable coefficients. For many classes of equations such approximations have already been constructed, however, the speed of their convergence to the exact solution has not been properly studied. We developed a program in Python 3 that allows to model a wide class of Chernoff approximations to a wide class of evolution equations on the real line. After that we select the heat equation (with already known exact solutions) as a simple yet informative model example for the study of the rate of convergence of Chernoff approximations. Examples illustrating the rate of convergence of Chernoff approximations to the solution of the Cauchy problem for the heat conduction equation are constructed in the paper. Numerically we show that for initial conditions that are smooth enough the order of approximation is equal to the order of Chernoff tangency of the Chernoff function used. We also consider not smooth enough initial conditions and show how Hölder class of initial condition is related to the rate of convergence. This method of study can be applied to general second order parabolic equation with variable coefficients by a slight modification of our Python 3 code, the full text of it is provided in the appendix to the paper.

Contents

1 Introduction

Chernoff approximations are a flexible and powerful tool of functional analysis [3, 4, 5], which can be used, in particular, to find numerically approximate solutions of some differential equations with variable coefficients, see [2, 14] for an introduction to this topic, and also Preliminaries section of the paper. For given linear evolution equation the method of Chernoff approximation generates a sequence of functions $u_n(t,x)$ that converge to the exact solution $u(t,x)$ of the equation studied. For arbitrary fixed moment of time t functions $x \longmapsto u(t,x)$ and $x \longmapsto u_n(t,x)$ are elements of some Banach space, and Chernoff's theorem guarantees that $\|u(t,\cdot) - u_n(t,\cdot)\| \to 0$ as $n \to \infty$.

To our current knowledge all contributions to a very young "theory of rates of convergence in Chernoff's theorem" can be found in [8, 19, 20, 7, 6] and references therein. These papers provide estimates for the rate of convergence under some conditions but if these conditions are not satisfied then one can say nothing about the quality of Chernoff approximations. There are also very few "practical" research papers [10, 16] that measure the speed of convergence in particular cases obtained via numerical simulations. In our research we continue contributions to this field of study.

We consider initial value problem for the heat equation

$$\begin{cases} u'_t(t,x) = u''_{xx}(t,x) \text{ for } t > 0, x \in \mathbb{R}^1 \\ u(0,x) = u_0(x) \text{ for } x \in \mathbb{R}^1 \end{cases} \tag{1}$$

which is a good model example because its bounded solution $u(t,x)$ is already known and given by the formula

$$u(t,x) = \int_{\mathbb{R}} \Phi(x-y,t)u_0(y)dy, \text{ where } \Phi(x,t) = (2\sqrt{\pi t})^{-1} \exp\left(\frac{-x^2}{4t}\right).$$

Then we obtain Chernoff approximations $u_n(t,x)$ to the exact solution $u(t,x)$ for $n = 1, 2, \ldots, 11$ and fixed time $t = 1/2$, and via numerical simulation and linear regression (ordinary least squares method) discover that

$$\sup_{x\in\mathbb{R}} |u(t,x) - u_n(t,x)| \approx \left(\frac{1}{n}\right)^{\beta}$$

with a reasonable accuracy ($R^2 > 0.98$). Coefficient $\beta > 0$ depends on the smoothness of initial condition u_0 and of the way of constructing the Chernoff approximations.

P.S.Prudnikov in 2020 studied [16] this question in a similar setting, but his approach does not allow a direct generalization. Meanwhile the simulation method that we use allows to study not only heat equation, but also equations with variable coefficients. Also we consider more initial conditions than were studied in [16].

Now let us provide necessary background on the topic to explain the notion of Chernoff tangency and Chernoff operator-valued function that are important to understand how we obtain Chernoff approximations $u_n(t,x)$.

2 Preliminaries

Let $\mathcal{F}$ be a Banach space. Let $\mathscr{L}(\mathcal{F})$ be a set of all bounded linear operators in $\mathcal{F}$. Suppose we have a mapping $V\colon [0,+\infty) \to \mathscr{L}(\mathcal{F})$, i.e. $V(t)$ is a bounded linear operator $V(t)\colon \mathcal{F} \to \mathcal{F}$ for each $t \geq 0$. The mapping V is called [5] a *C_0-semigroup*, or *a strongly continuous one-parameter semigroup of operators* iff it satisfies the following conditions:

1) $V(0)$ is the identity operator I, i.e. $\forall \varphi \in \mathcal{F} : V(0)\varphi = \varphi$;

2) V maps the addition of numbers in $[0,+\infty)$ into the composition of operators in $\mathscr{L}(\mathcal{F})$, i.e. $\forall t \geq 0, \forall s \geq 0 : V(t+s) = V(t) \circ V(s)$, where for each $\varphi \in \mathcal{F}$ the notation $(A \circ B)(\varphi) = A(B(\varphi)) = AB\varphi$ is used;

3) V is continuous with respect to the strong operator topology in $\mathscr{L}(\mathcal{F})$, i.e. $\forall \varphi \in \mathcal{F}$ function $t \longmapsto V(t)\varphi$ is continuous as a mapping $[0,+\infty) \to \mathcal{F}$.

The definition of a *C_0-group* is obtained by the substitution of $[0,+\infty)$ by $\mathbb{R}$ in the paragraph above.

It is known [5] that if $(V(t))_{t\geq 0}$ is a C_0-semigroup in Banach space $\mathcal{F}$, then the set

$$\left\{\varphi \in \mathcal{F} : \exists \lim_{t\to+0} \frac{V(t)\varphi - \varphi}{t}\right\} \overset{denote}{=} Dom(L)$$

is a dense linear subspace in $\mathcal{F}$. The operator L defined on the domain $Dom(L)$ by the equality

$$L\varphi = \lim_{t\to+0} \frac{V(t)\varphi - \varphi}{t}$$

is called *an infinitesimal generator* (or just *generator* to make it shorter) of the C_0-semigroup $(V(t))_{t\geq 0}$, and notation $V(t) = e^{tL}$ is widely used.

One of the reasons for the study of C_0-semigroups is their connection with differential equations. If Q is a set, then the function $u\colon [0,+\infty) \times Q \to \mathbb{R}$, $u\colon (t,x) \longmapsto u(t,x)$ of two variables (t,x) can be considered as a function $u\colon t \longmapsto [x \longmapsto u(t,x)]$ of one variable t with values in the space of functions of the variable x. If $u(t,\cdot)\in\mathcal{F}$ then one can define $Lu(t,x) = (Lu(t,\cdot))(x)$. If there exists a C_0-semigroup $(e^{tL})_{t\geq 0}$ then the Cauchy problem for a linear evolution equation

$$\begin{cases} u_t'(t,x) = Lu(t,x) \text{ for } t>0, x\in Q \\ u(0,x) = u_0(x) \text{ for } x\in Q \end{cases} \tag{2}$$

has a unique (in sense of $\mathcal{F}$, where $u(t,\cdot)\in\mathcal{F}$ for every $t\geq 0$) solution

$$u(t,x) = (e^{tL}u_0)(x)$$

depending on u_0 continuously. Compare also different meanings of the solution [5], including mild solution which solves the corresponding integral equation. Note that if there exists a strongly continuous group $(e^{tL})_{t\in\mathbb{R}}$ then in the Cauchy problem the equation $u_t'(t,x) = Lu(t,x)$ can be considered not only for $t>0$, but for $t\in\mathbb{R}$, and the solution is provided by the same formula $u(t,x) = (e^{tL}u_0)(x)$.

Definition 1 (*Introduced in [13]*). Let us say that C is *Chernoff-tangent* to L iff the following conditions of Chernoff tangency (CT) hold:

(CT0). Let $\mathcal{F}$ be a Banach space, and $\mathscr{L}(\mathcal{F})$ be a space of all linear bounded operators in $\mathcal{F}$. Suppose that we have an operator-valued function $C\colon [0,+\infty)\to\mathscr{L}(\mathcal{F})$, or, using other words, we have a family $(C(t))_{t\geq 0}$ of linear bounded operators in $\mathcal{F}$. Closed linear operator $L\colon Dom(L)\to\mathcal{F}$ is defined on the linear subspace $Dom(L)\subset\mathcal{F}$ which is dense in $\mathcal{F}$.

(CT1) Function $t\longmapsto C(t)f\in\mathcal{F}$ is continuous for each $f\in\mathcal{F}$.

(CT2) $C(0)=I$, i.e. $C(0)f = f$ for each $f\in\mathcal{F}$.

(CT3) There exists such a dense subspace $\mathcal{D}\subset\mathcal{F}$ that for each $f\in\mathcal{D}$ there exists a limit

$$C'(0)f = \lim_{t\to 0}\frac{C(t)f - f}{t}.$$

(CT4) The closure of the operator $(C'(0),\mathcal{D})$ is equal to $(L, Dom(L))$.

Remark 1. Let us consider one-dimensional example $\mathcal{F} = \mathscr{L}(\mathcal{F}) = \mathbb{R}$. Then $g\colon[0,+\infty)\to\mathbb{R}$ is Chernoff-tangent to $l\in\mathbb{R}$ iff $g(t) = 1 + tl + o(t)$ as $t\to +0$.

Theorem 1 (P. R. Chernoff (1968), see [5, 3]). Let $\mathcal{F}$ and $\mathscr{L}(\mathcal{F})$ be as above. Suppose that the operator $L\colon\mathcal{F}\supset Dom(L)\to\mathcal{F}$ is linear and closed, and function C takes values in $\mathscr{L}(\mathcal{F})$. Suppose that these assumptions are fulfilled:

(E) There exists a C_0-semigroup $(e^{tL})_{t\geq 0}$ with the infenitesimal generator $(L, Dom(L))$.

(CT) C is Chernoff-tangent to $(L, Dom(L))$.

(N) There exists such a number $\omega\in\mathbb{R}$, that $\|C(t)\|\leq e^{\omega t}$ for all $t\geq 0$.

Then for each $f\in\mathcal{F}$ we have $(C(t/n))^n f\to e^{tL}f$ as $n\to\infty$ with respect to norm in $\mathcal{F}$ uniformly with respect to $t\in[0,T]$ for each $T>0$, i.e.

$$\lim_{n\to\infty}\sup_{t\in[0,T]}\left\|e^{tL}f - (C(t/n))^n f\right\| = 0.$$

Remark 2. In our one-dimensional example ($\mathcal{F} = \mathscr{L}(\mathcal{F}) = \mathbb{R}$) the Chernoff theorem says that $e^{tl} = \lim_{n\to\infty} g(t/n)^n = \lim_{n\to\infty}(1 + tl/n + o(t/n))^n$, which is a simple fact of calculus.

Definition 2. Let $\mathcal{F}, \mathscr{L}(\mathcal{F}), L$ be as above. If C is Chernoff-tangent to L and the equation $\lim_{n\to\infty}\sup_{t\in[0,T]}\left\|e^{tL}f - (C(t/n))^n f\right\| = 0$ holds, then C is called *a Chernoff function* for the operator L, and the $(C(t/n))^n f$ is called *a Chernoff approximation expression* to $e^{tL}f$.

Remark 3. If L is a linear bounded operator in $\mathcal{F}$, then $e^{tL} = \sum_{k=0}^{+\infty}(tL)^k/k!$ where the series converges in the usual operator norm topology in $\mathscr{L}(\mathcal{F})$. When L is not bounded (such as Laplacian and many other differential operators), expressing $(e^{tL})_{t\geq 0}$ in terms of L is not an easy problem that is equivalent to the problem of finding (for each $u_0 \in \mathcal{F}$) the $\mathcal{F}$-valued function U that solves the Cauchy problem $U'(t) = LU(t); U(0) = u_0$. If one finds this solution, then e^{tL} is obtained for each $u_0 \in \mathcal{F}$ and each $t \geq 0$ in the form $e^{tL}u_0 = U(t)$.

Remark 4. In the definition of the Chernoff tangency the family $(C(t))_{t\geq 0}$ usually does not have a semigroup composition property, i.e. $C(t_1 + t_2) \neq C(t_1)C(t_2)$, while $(e^{tL})_{t\geq 0}$ has it: $e^{t_1 L}e^{t_2 L} = e^{(t_1+t_2)L}$. However, each C_0-semigroup $(e^{tL})_{t\geq 0}$ is Chernoff-tangent to its generator L and appears to be it's Chernoff function. When coefficients of the operator L are variable, usually there is no simple formula for e^{tL} due to the remark 3. On the other hand, even in this case one can find rather simple formula to construct Chernoff function C for the operator L, because there is no need to worry about the composition property, and then obtain e^{tL} in the form $e^{tL} = \lim_{n\to\infty} C(t/n)^n$ via the Chernoff theorem.

3 Numerical simulation results

3.1 Problem setting

Definition 3. We say that operator-valued function C is *Chernoff-tangent of order k* to operator L iff C is Chernoff-tangent to L in the sense of definition 1 and the following condition (CT3-k) holds:

There exists such a dense subspace $\mathcal{D} \subset \mathcal{F}$ that for each $f \in \mathcal{D}$ we have

$$C(t)f = \left(I + tL + \frac{1}{2}t^2L^2 + \ldots + \frac{1}{k!}t^kL^k\right) f + o(t^k) \text{ as } t \to 0.$$

Remark 5. It is clear that for $k = 1$ condition (CT3-k) becomes just (CT3). For the semigroup $C(t) = e^{tL}$ condition (CT3-k) holds for all $k = 1, 2, 3, \ldots$ So one can expect that the bigger k is the better rate of convergence $C(t/n)^n f \to e^{tL}f$ as $n \to \infty$ will be, if f belongs to the space D. This idea was proposed in [12], where two conjectures about the convergence speed were formulated explicitly, and one of them were recently proved in [7, 6]. For initial conditions that are good enough and t fixed, Chernoff function with Chernoff tangency of order k by conjecture should provide $\|u(t,\cdot) - u_n(t,\cdot)\| = O(1/n^k)$ as $n \to \infty$. However, if $f \notin D$ then nothing is known on the rate of convergence. In the present paper we are starting to fill this gap for operator L given by $(Lf)(x) = f''(x)$ for all $x \in \mathbb{R}$ and all bounded, infinitely smooth functions

$f\colon \mathbb{R} \to \mathbb{R}$, and $k = 1, 2$.

Problem setting. In the initial value problem (2) consider $Q = \mathbb{R}$, and Banach space $\mathcal{F} = UC_b(\mathbb{R})$ of all bounded, uniformly continuous functions $f\colon \mathbb{R} \to \mathbb{R}$ endowed with the uniform norm $\|f\| = \sup_{x\in\mathbb{R}} |f(x)|$. Consider operator L given by $(Lf)(x) = f''(x)$ for all $x \in \mathbb{R}$ and all $f \in D = C_b^\infty(\mathbb{R})$ of all infinitely smooth functions $\mathbb{R} \to \mathbb{R}$ that are bounded with all the derivatives. Then (2) reads as (1). Cauchy problem (1) is a constant (one, zero, zero) coefficients particular case of the Cauchy problem considered in [15], and the corresponding Chernoff function was found in [15]. The particular case of this Chernoff function reads as

$$(G(t)f)(x) = \frac{1}{2}f(x) + \frac{1}{4}f(x + 2\sqrt{t}) + \frac{1}{4}f(x - 2\sqrt{t})$$

where we write $G(t)$ instead of $C(t)$ in order to show that $C(t)$ is a general abstract Chernoff function for some operator L, meanwhile $G(t)$ is this particular above-given Chernoff function for operator d^2/dx^2. It was proved in [15] that $G(t)$ is first order Chernoff-tangent to d^2/dx^2.

A.Vedenin (see [19]) proposed another Chernoff function for operator L considered in [15], and the constant coefficient particular case of this operator is d^2/dx^2. The particular case of the Chernoff function obtained by A.Vedenin reads as

$$(S(t)f)(x) = \frac{2}{3}f(x) + \frac{1}{6}f(x + \sqrt{6t}) + \frac{1}{6}f(x - \sqrt{6t}),$$

and it was proved by A.Vedenin that $S(t)$ is second order Chernoff-tangent to d^2/dx^2.

In the paper we study how $\sup_{x\in\mathbb{R}} |u(t,x) - u_n(t,x)|$ depends on n while $t = 1/2$ is fixed and $u_n(t,x)$ is given by

$$u_n(t,x) = (C(t/n)^n u_0)(x)$$

where $C \in \{G, S\}$, $C(t/n)$ is obtained by substitution of t by t/n in the formula that defines $C(t)$, and $C(t/n)^n = C(t/n)C(t/n)\ldots C(t/n)$ is a composition of n copies of linear bounded operator $C(t/n)$. We consider several initial conditions u_0 that are all Hölder continuous (hence all belong to the $UC_b(\mathbb{R})$ space) but have different Hölder exponents. Then we remark how the rate of tending of $\sup_{x\in\mathbb{R}} |u(t,x) - u_n(t,x)|$ to zero depends on these Hölder exponents and the order of Chernoff tangency (which is 1 for $G(t)$, and 2 for $S(t)$).

Comments on computational techniques. Calculations were performed in the Python 3 environment using a program we wrote and which is available in the Appendix. All measurements, for the sake of reducing computational complexity, for each value of n (varying from 1 to 11) were carried out for 1000 points uniformly dividing the segment $[-\pi, \pi]$ or $[-2\pi, 2\pi]$. Initial conditions of the form $u_0(x) = |\sin x|^\alpha$ for various $\alpha \in \{9/2, 7/2, 5/2, 3/2, 1, 3/4, 1/2, 1/4\}$, like any of Chernoff approximations based on them, are periodic functions. So, the standard norm in $UC_b(\mathbb{R})$, namely

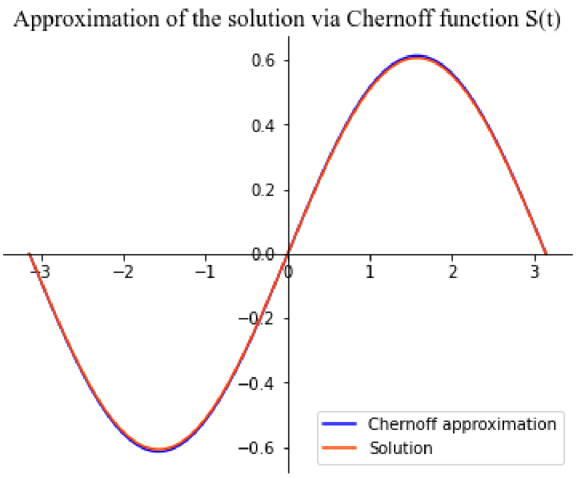
$$d = \|u_n(t,\cdot) - u(t,\cdot)\| = \sup_{x\in\mathbb{R}} |u_n(t,x) - u(t,x)|,$$

where u is the exact solution of (1) and u_n is the Chernoff approximation, is reached at the interval corresponding to the period.

The program code was written with the possibility to set any operator and any initial condition, i.e. without simplifying Chernoff functions and using binomial coefficients, in contrast to the work [16] published earlier. Moreover, the initial condition does not necessarily have to be a smooth function. The number of iterations is not limited to 11, the value n can be changed, both upward and downward. We have chosen the optimal value n since the program is very time consuming: via Jupyter Notebook 6.1.4 Anaconda 3 Python 3.8.3 set on personal computer with Windows 10, CPU Intel Core i5-1035G1, 1.0-3.6 GHz, 8 Gb RAM it takes about 20 minutes to complete the program for all initial conditions with construction of graphs for them. At the research stage of the new method (Chernoff approximations) this is acceptable, but in the future, of course, the code will be optimized for a better speed, since this is important in practice. Our goal is to continue research and in the future write a library that allows to solve partial derivative equations in this way.

3.2 Approximations for initial condition $u_0(x) = \sin(x)$

Let us first analyze the approximations for the initial condition $u_0(x) = \sin x$.



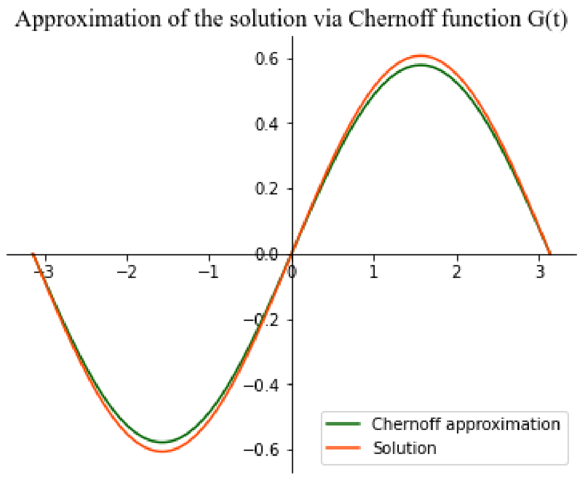


fig. 1.1, $n = 1$, $u_0(x) = \sin x$, $t = \frac{1}{2}$

Figure 1.1 shows the exact solution, which coincides with the graph of the function $y = e^{-1/2} \sin x$, and approximate solutions for the functions $S(t)$ (left) and $G(t)$ (right) at $n = 1$. The initial condition $u_0 = \sin x$ is very good, since its derivatives of any order exist, have no discontinuities and are bounded. And already at $n = 1$ the function $S(t)$ gives a good approximation.

Figure 1.2 below shows plots of the decreasing error of Chernoff approximations as a function of n, where $1 \leq n \leq 11$. On the left are plots of decreasing error for Chernoff functions $S(t)$ (in blue) and $G(t)$ (in green) in regular scale, and on the right – the same plots in logarithmic scale. The graph in the logarithmic scale allows us to estimate how much the convergence rate for the function $G(t)$ is less than the convergence rate for the function $S(t)$. Here and through all the paper we use the following notation:

$$d = \|u_n(t,\cdot) - u(t,\cdot)\| = \sup_{x\in\mathbb{R}} |u_n(t,x) - u(t,x)|.$$

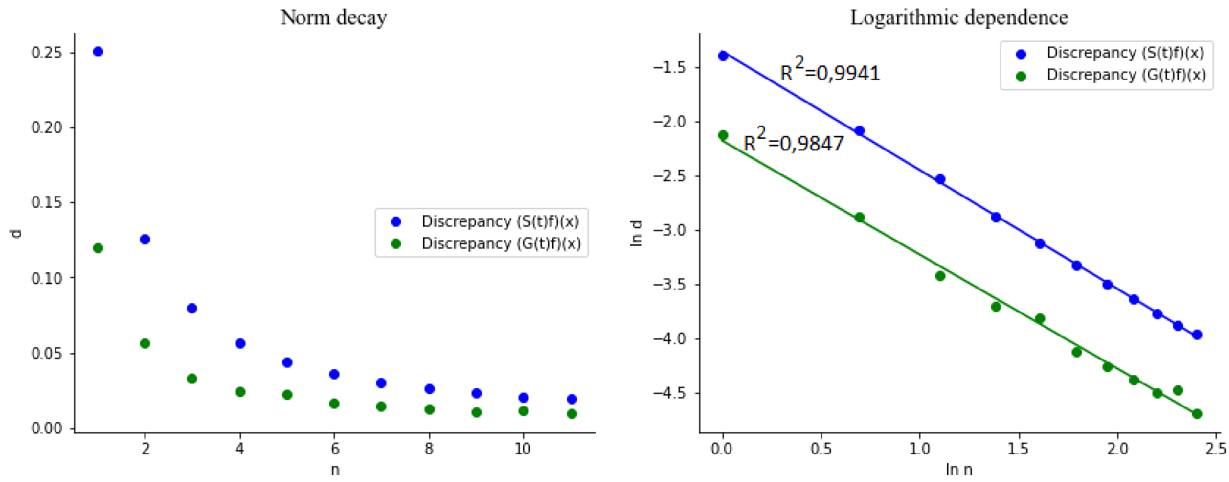


fig. 1.2, $1 \leq n \leq 11$, $u_0(x) = \sin x$, $t = \frac{1}{2}$

You can see that the points on the right graph lie on the straight lines with good accuracy. Using the method of least squares (in Excel) we found the equations of these lines. Rounding off the coefficients, we see that for the blue line the equation is as follows:
$\ln(d) = -2.092\ln(n) - 5.0671$, i.e. $d = n^{-2.092}e^{-5.0671} = \frac{0.0063}{n^{2.092}}$.

Similarly, for the green line, the equation $\ln(d) = -1.0416\ln(n) - 3.5796$, i.e. $d = n^{-1.0416}e^{-3.5796} = \frac{0.0279}{n^{1.0416}}$.

Using the same approach, we study the behavior of the error for other initial conditions.

3.3 Approximations for initial condition $u_0(x) = |\sin x|$

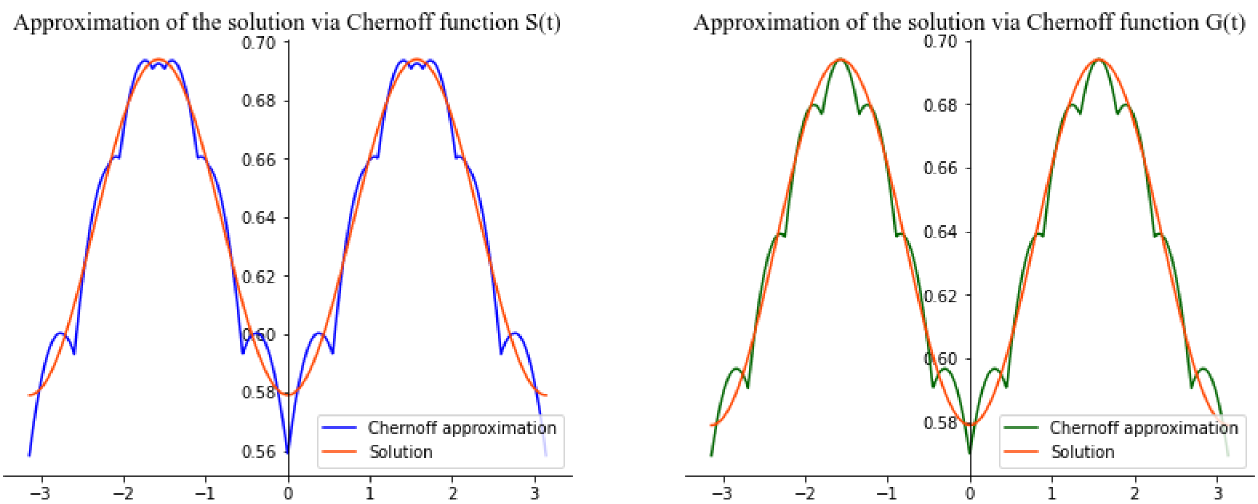


fig. 2.1, $n = 10$, $u_0(x) = |\sin x|$, $t = \frac{1}{2}$

Figure 2.1 shows two graphs of the approximate solution for the functions we are studying, at $n = 10$, and the exact solution under the initial condition $u_0(x) = |\sin x|$

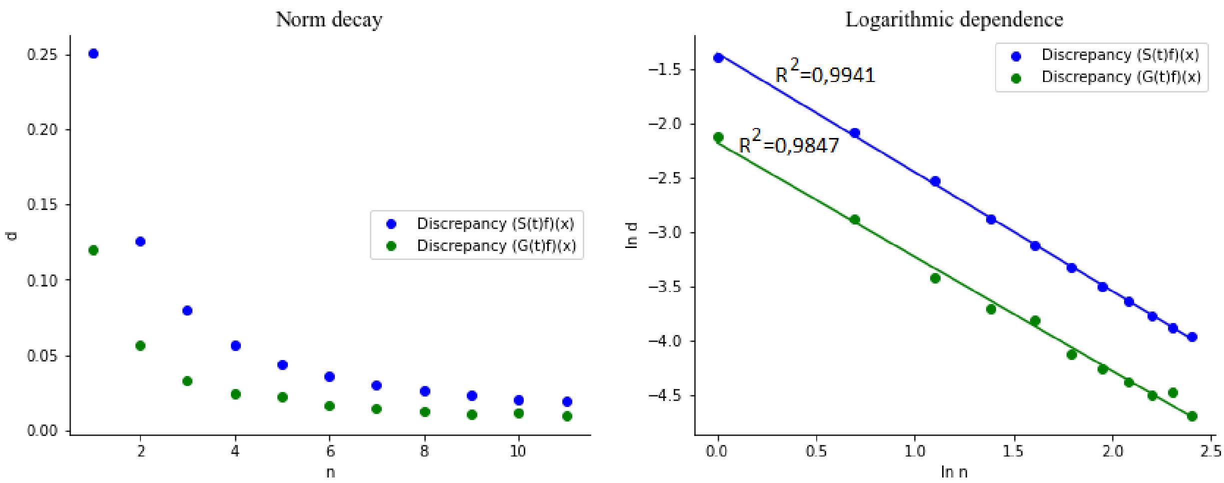


fig. 2.2, $1 \leq n \leq 11$, $u_0(x) = |\sin x|$, $t = \frac{1}{2}$

Rounding off the coefficients, we see that for the blue line (see Fig. 2.2) the equation is as follows: $\ln(d) = -1.0948 \ln(n) - 1.355$, i.e. $d = n^{-1.0948} e^{-1.355} = \frac{0.2579}{n^{1.0948}}$.

Similarly, for the green line (see Figure 2.2), the equation $\ln(d) = -1.0508 \ln(n) - 2.1782$, i.e. $d = n^{-1.0508} e^{-2.1782} = \frac{0.1132}{n^{1.0508}}$.

Consider the new initial condition $u_0(x) = \sqrt{|\sin x|}$.

3.4 Approximations for initial condition $u_0(x) = \sqrt{|\sin x|}$

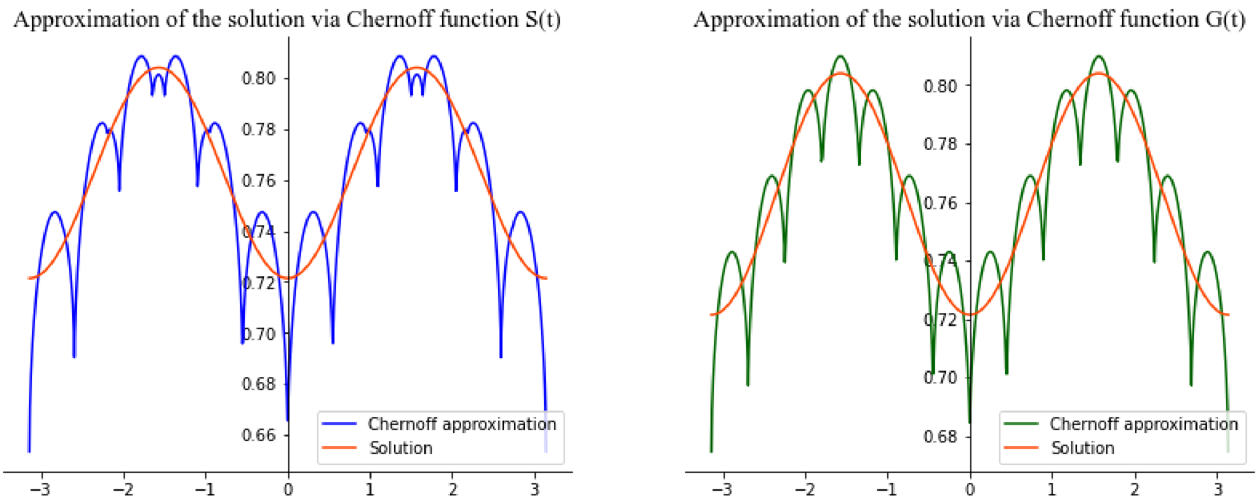


fig. 3.1, $n = 10$, $u_0(x) = \sqrt{|\sin x|}$, $t = \frac{1}{2}$

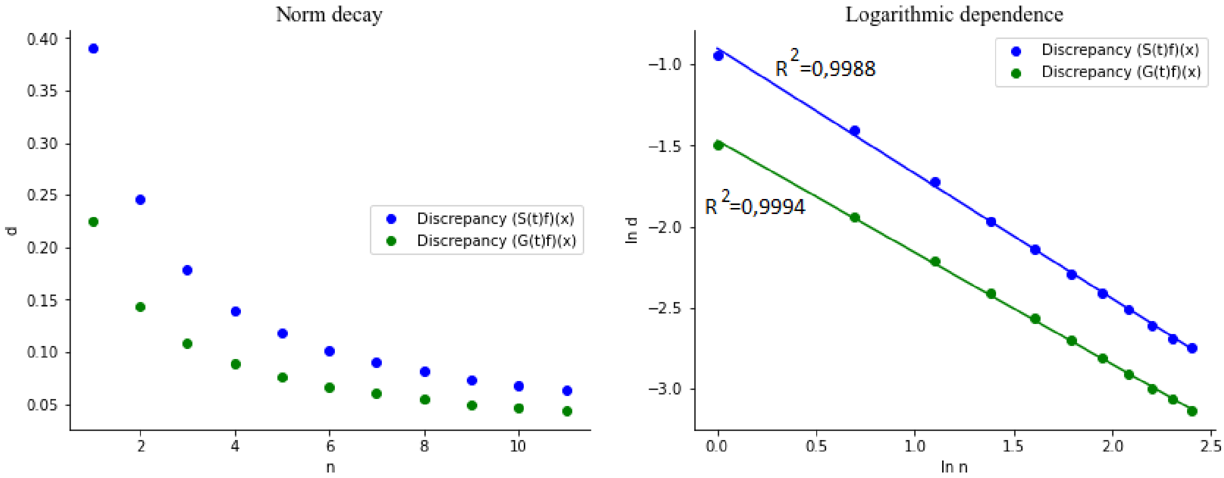


fig. 3.2, $1 \leq n \leq 11$, $u_0(x) = \sqrt{|\sin x|}$, $t = \frac{1}{2}$

For the blue line (see Fig. 3.2, right) the equation is as follows:
$\ln(d) = -0.7723\ln(n) - 0.9013$, т.е. $d = n^{-0.7723}e^{-0.9013} = \frac{0.4060}{n^{0.7723}}$.

Similarly, for the green line (see Fig. 3.2, right) the equation $\ln(d) = -0.6905\ln(n) - 1.4709$, т.е. $d = n^{-0.6905}e^{-1.4709} = \frac{0.2297}{n^{0.6905}}$.

3.5 Approximations for initial condition $u_0(x) = \sqrt[4]{|\sin x|}$

Note that all special cases $\sqrt[\alpha]{|\sin x|}$, where $\alpha < 1$, are similar to the already considered cases. In fact, consider $\alpha = 1/4$.

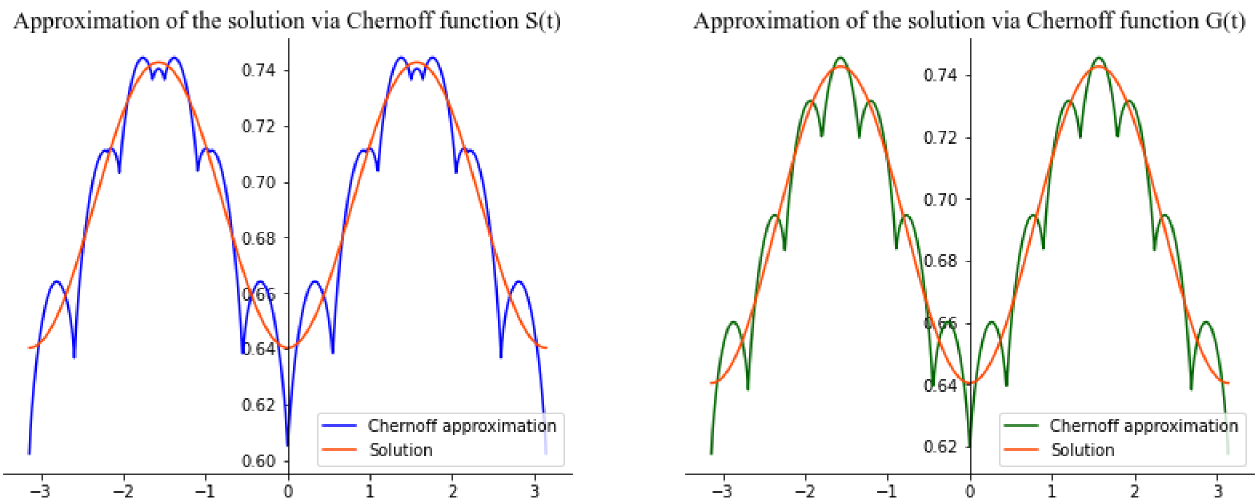


fig. 4.1, $n = 10$, $u_0(x) = \sqrt[4]{|\sin x|}$, $t = \frac{1}{2}$

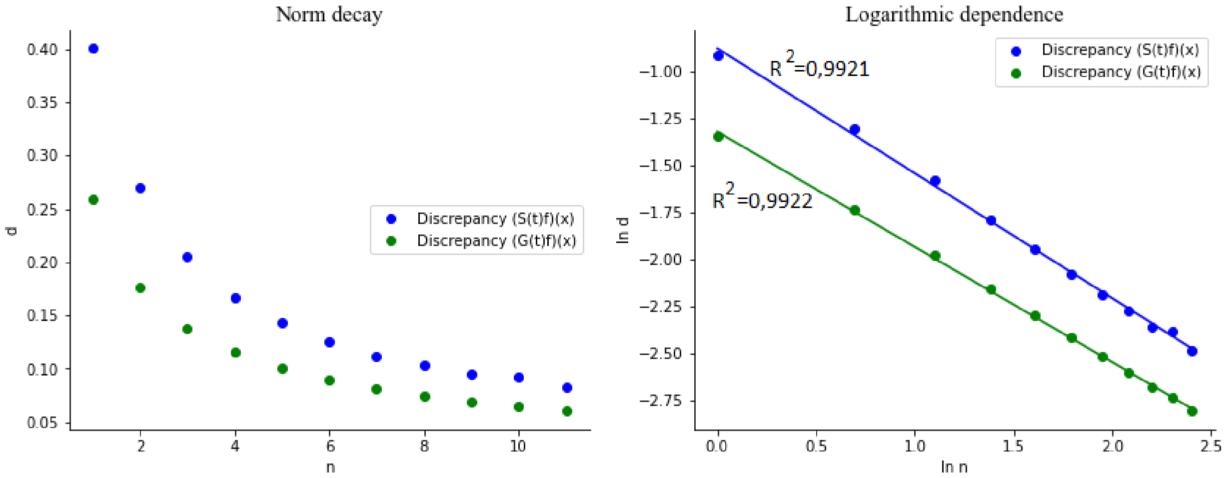


fig. 4.2, $1 \le n \le 11$, $u_0(x) = \sqrt[4]{|\sin x|}$, $t = \frac{1}{2}$

Rounding the coefficients, we see that for the blue line (see Figure 4.2, right) the equation is as follows: $\ln(d) = -0.6653\ln(n) - 0.8789$, $d = n^{-0.6653}e^{-0.8789} = \frac{0.4152}{n^{0.6653}}$.

Similarly, for the green line (see Fig. 4.2, right) the equation $\ln(d) = -0.6138\ln(n) - 1.3228$, т.е. $d = n^{-0.6138}e^{-1.3228} = \frac{0.2664}{n^{0.6138}}$.

3.6 Approximations for initial condition $u_0(x) = |\sin(x)|^{3/2}$

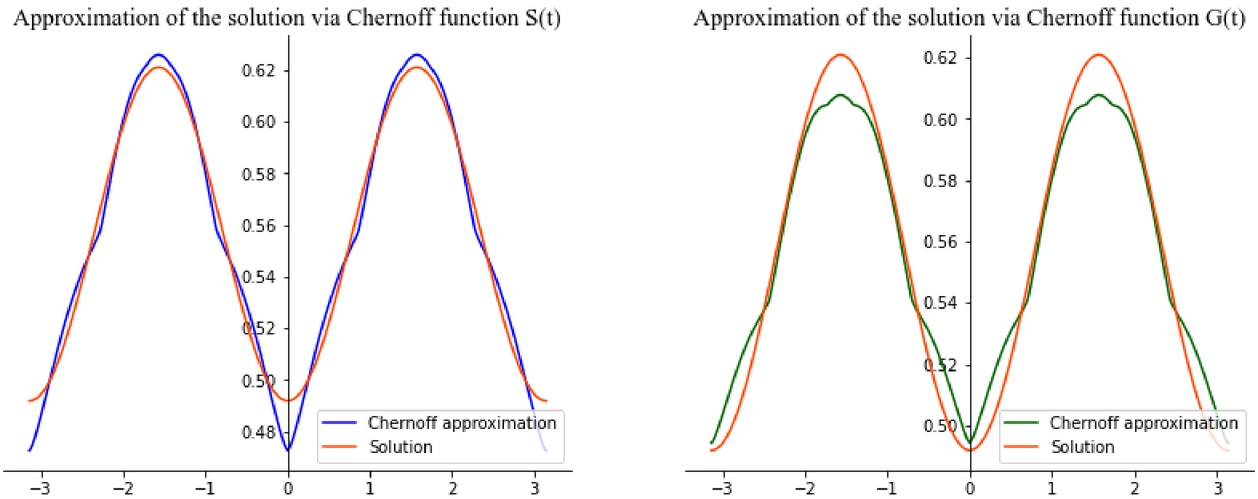


fig. 5.1, $n = 4$, $u_0(x) = |\sin(x)|^{3/2}$, $t = \frac{1}{2}$

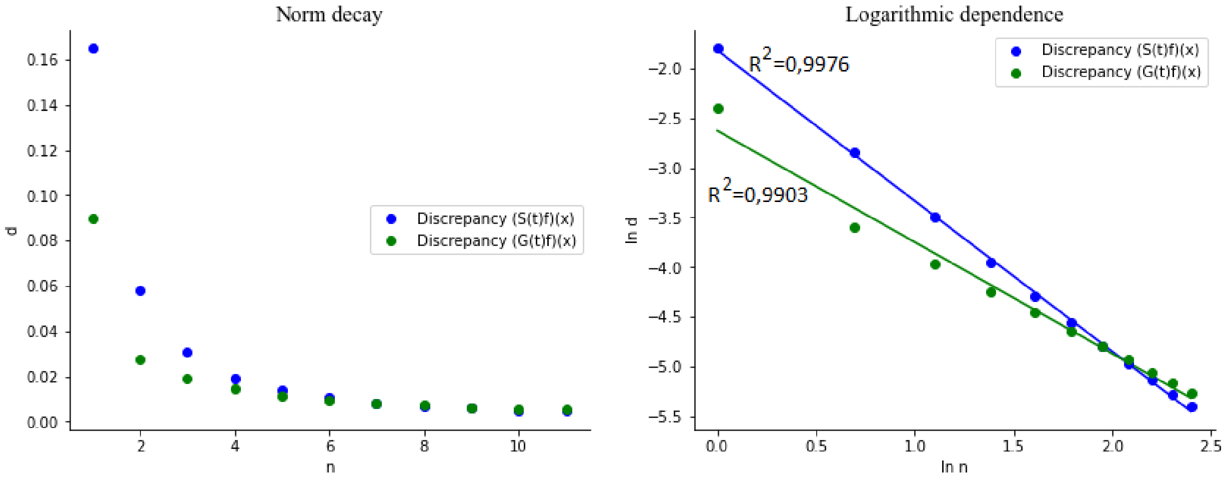


fig. 5.2, $1 \leq n \leq 11$, $u_0(x) = |\sin(x)|^{3/2}$, $t = \frac{1}{2}$

The line (green) corresponding to the decreasing error of the function $G(t)$ in the logarithmic scale was constructed without taking into account $n = 1$.

For the green line (see Fig. 5.2, right) the equation $\ln(d) = -0.9785 \ln(n) - 2.8973$, i.e. $d = n^{-0.9785} e^{-2.8973} = \frac{0.0552}{n^{0.9785}}$.

Similarly, for the blue line (see Figure 5.2), the equation is as follows: $\ln(d) = -1.5109 \ln(n) - 1.8234$, i.e. $d = n^{-1.5109} e^{-1.8234} = \frac{0.1615}{n^{1.5109}}$.

As can be seen from Figure 5.2, the difference between the error decay rates using Chernoff functions $S(t)$ and $G(t)$ for $u_0(x) = |\sin(x)|^{3/2}$ is larger than for $u_0(x) = |\sin x|$. This is due to the greater smoothness of $u_0(x) = |\sin(x)|^{3/2}$.

3.7 Approximations for initial condition $u_0(x) = e^{-|x|}$

Let us consider a non-smooth and non-periodic function $e^{-|x|}$ as an initial condition.

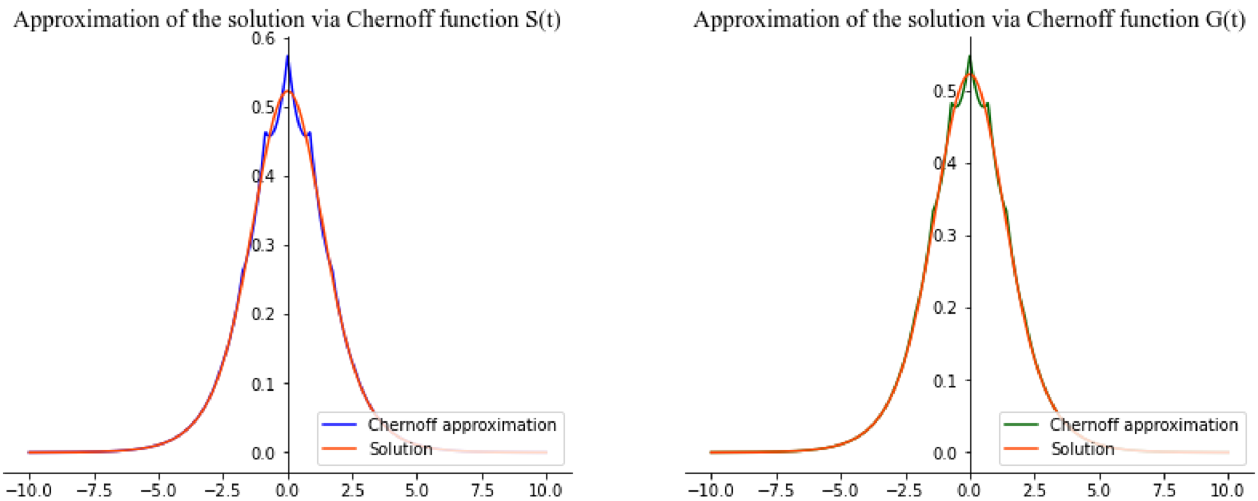


fig. 6.1, $n = 4$, $u_0(x) = e^{-|x|}$, $t = \frac{1}{2}$

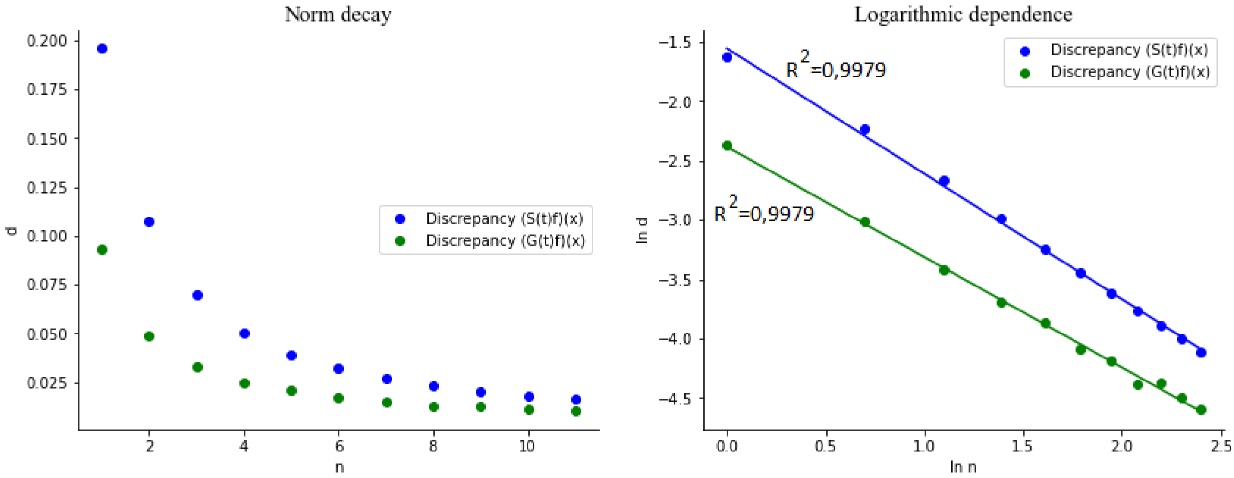


fig. 6.2, $1 \le n \le 11$, $u_0(x) = e^{-|x|}$, $t = \frac{1}{2}$

Figures 6.1 and 6.2 show plots of the exact solution, approximations to the solution, and rates of convergence of the error to zero. As can be seen, the result is similar: the convergence rate of the function $S(t)$ is higher than that of $G(t)$, but the order of convergence is approximately the same, as can be seen from the fact that the lines are almost parallel.

For the green line (see Fig. 6.2, right), the equation is as follows: $\ln(d) = -0.9294 \ln(n) - 2.3832$, i.e. $d = n^{-0.9294} e^{-2.3832} = \frac{0.0923}{n^{0.9294}}$.

Similarly, for the blue line (see Figure 6.2) the equation is as follows: $\ln(d) = -1.056 \ln(n) - 1.5543$, i.e. $d = n^{-1.056} e^{-1.5543} = \frac{0.2113}{n^{1.5543}}$.

3.8 Approximations for initial condition $u_0(x) = |\sin(x)|^{5/2}$

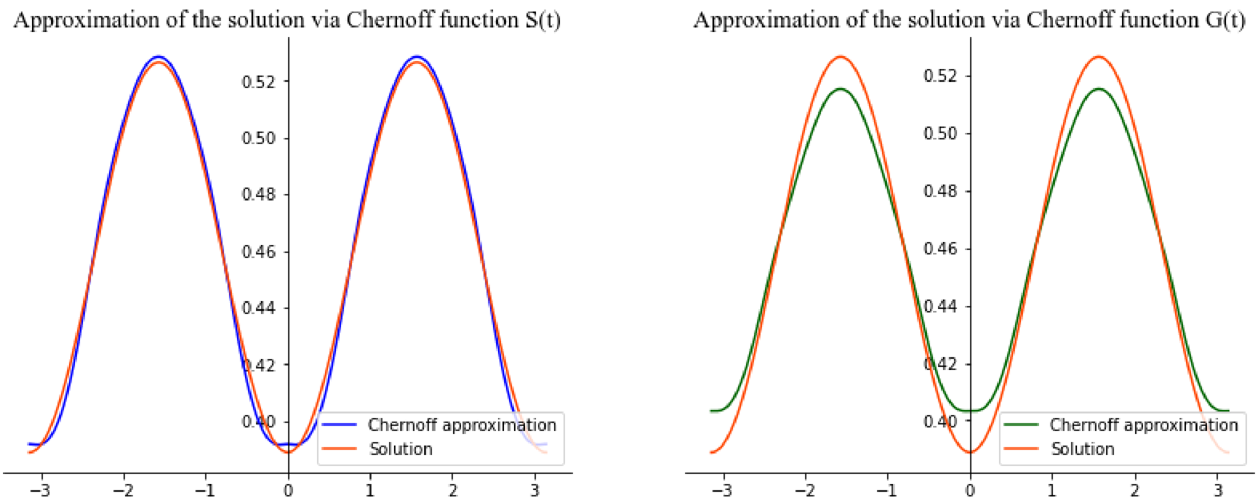


fig. 7.1, $n = 4$, $u_0(x) = |\sin(x)|^{5/2}$, $t = \frac{1}{2}$

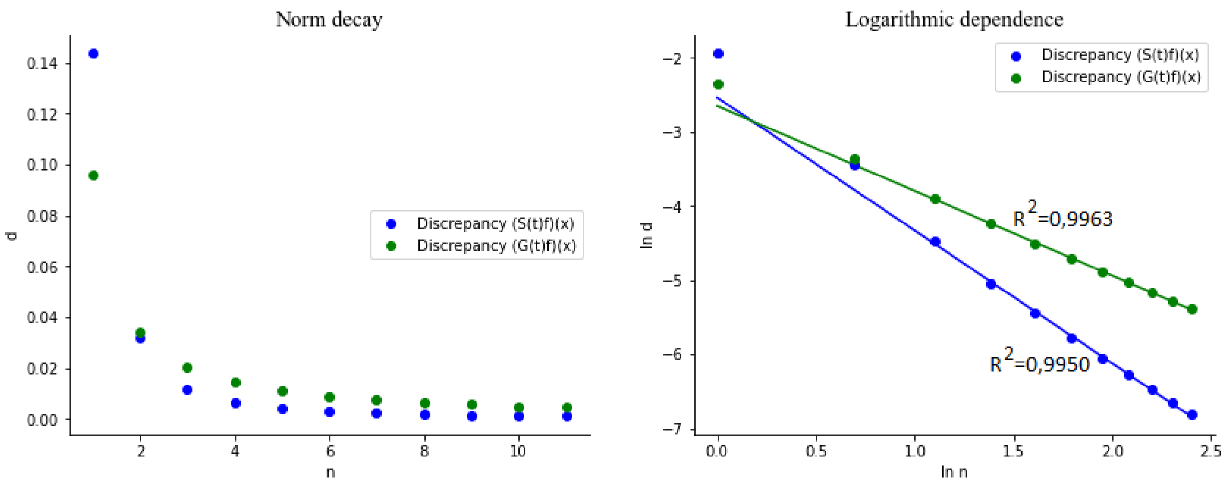


fig. 7.2, $1 \leq n \leq 11$, $u_0(x) = |\sin(x)|^{5/2}$, $t = \frac{1}{2}$

The lines (green and blue) corresponding to the decreasing error of the functions $G(t)$ and $S(t)$ in the logarithmic scale was constructed without taking into account $n = 1$ and $n = 2$.

3.9 Approximations for initial condition $u_0(x) = |\sin(x)|^{7/2}$

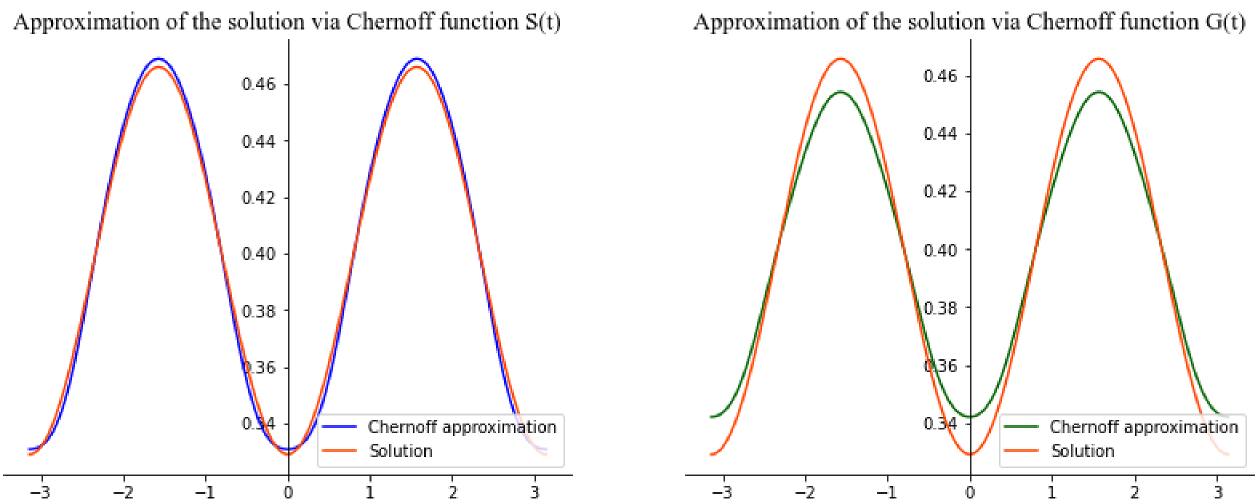


fig. 8.1, $n = 4$, $u_0(x) = |\sin(x)|^{7/2}$, $t = \frac{1}{2}$

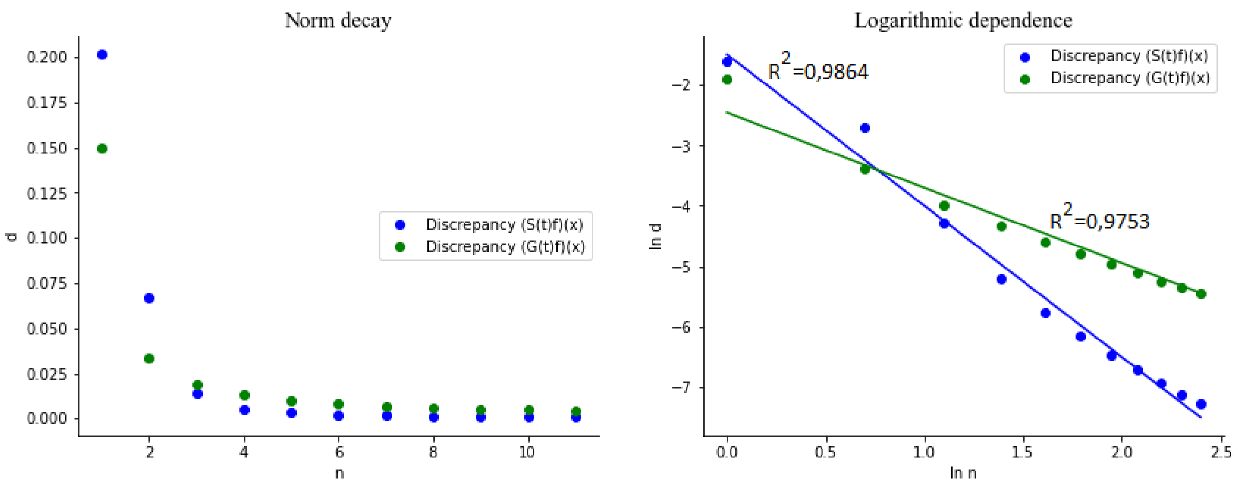


fig. 8.2, $1 \leq n \leq 11$, $u_0(x) = |\sin(x)|^{7/2}$, $t = \frac{1}{2}$

The line (green) corresponding to the decreasing error of the function $G(t)$ in the logarithmic scale was constructed without taking into account $n = 1$ and $n = 2$.

3.10 Approximations for initial condition $u_0(x) = |\sin(x)|^{9/2}$

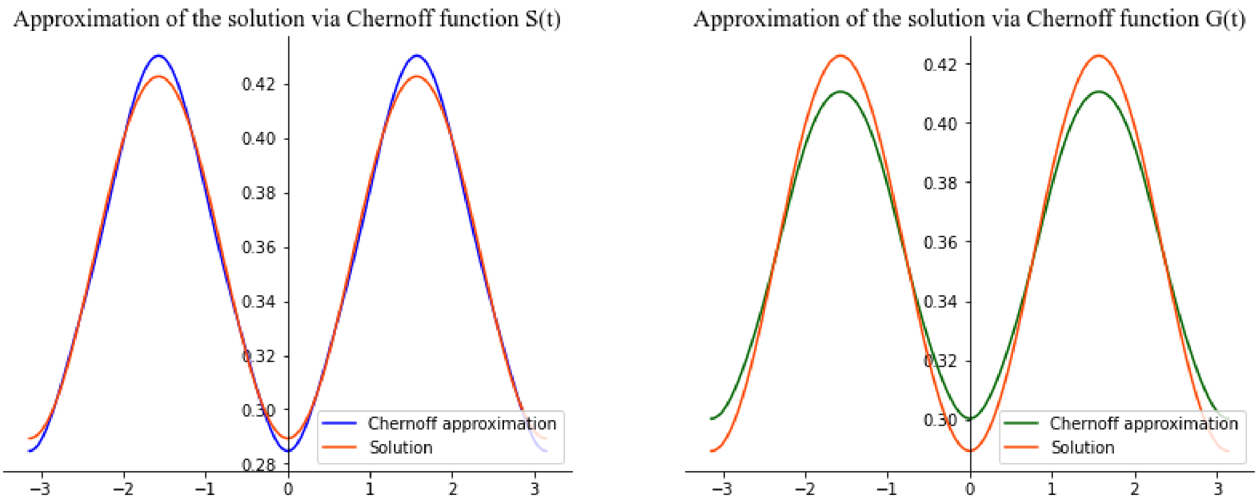


fig. 9.1, $n = 4$, $u_0(x) = |\sin(x)|^{9/2}$, $t = \frac{1}{2}$

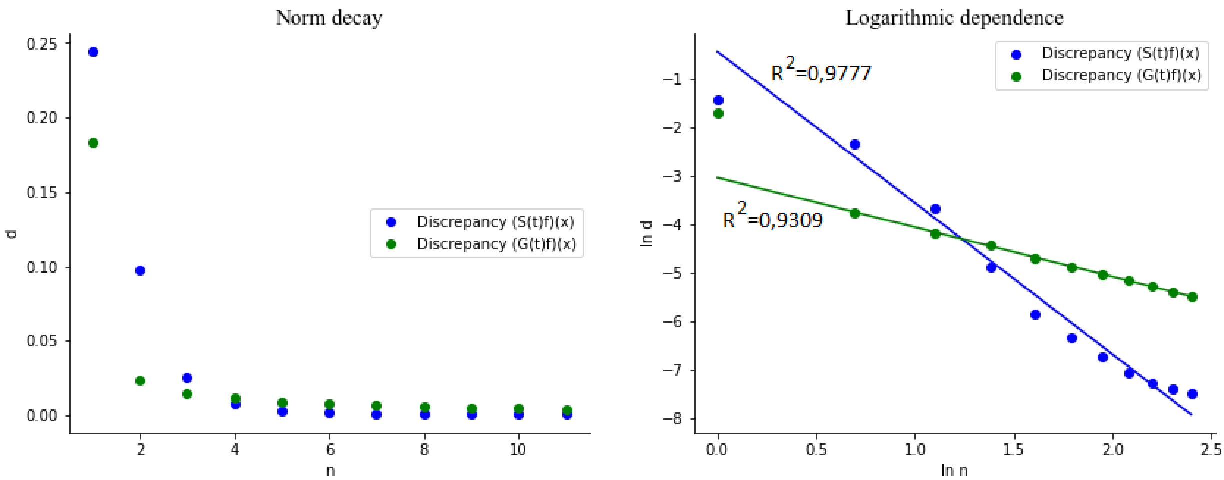


fig. 9.2, $1 \leq n \leq 11$, $u_0(x) = |\sin(x)|^{9/2}$, $t = \frac{1}{2}$

The line (green) corresponding to the decreasing error of the function $G(t)$ in the logarithmic scale was constructed without taking into account $n = 1$ and $n = 2$.

4 Discussion

The table below shows experimentally (using simulation in Python 3) the orders of decreasing of error depending on the smoothness class of the initial condition and the Chernoff function.

The smoothness class of the initial condition u_0	**Order of decreasing error on the Chernoff function $G(t)$, which has the 1st order of the Chernoff tangent to the operator $L = \frac{d^2}{dx^2}$**	**Order of decreasing error on the Chernoff function $S(t)$, which has the 2nd order of tangency by Chernoff to the operator $L = \frac{d^2}{dx^2}$**
C^∞, i.e. all derivatives exist and are bounded, $u_0(x) = \sin(x)$	-1.0416	-2.092
$C^{4\frac{1}{2}}$, the first, second, third, and fourth derivatives exist and are bounded, and the fifth is Hölder with a Hölder exponent 1/2, $u_0(x) = \lvert\sin(x)\rvert^{9/2}$	-1.0212, the regression was done without $n = 1$, $n = 2$	-3.1219, but the points do not fit well on a straight line, so the number is uninformative
$C^{3\frac{1}{2}}$, the first, second, and third derivatives exist and are bounded, and the fourth is Hölder with Hölder exponent 1/2, $u_0(x) = \lvert\sin(x)\rvert^{7/2}$	-1.4013,regression was done without considering $n = 1$, $n = 2$, but the points do not lie well on the line, so the number is uninformative	-2.5045, but the points do not lie well on the line, so the number is uninformative
$C^{2\frac{1}{2}}$, the first and second derivatives exist and are bounded, and the third is Hölder with Hölder exponent 1/2, $u_0(x) = \lvert\sin(x)\rvert^{5/2}$	-1.1433, regression was done without considering $n = 1$, $n = 2$	-1.7923, regression was done without considering $n = 1$, $n = 2$
$C^{1\frac{1}{2}}$, the first derivative exists and is bounded, and the second derivative with a Hölder index of 1/2, $u_0(x) = \lvert\sin(x)\rvert^{3/2}$	-0.9785, the regression was done without considering $n = 1$	-1.5109
H^1, the Hölder with the Hölder exponent 1, $u_0(x) = \lvert\sin(x)\rvert$	-1.0508	-1.0948
H^1,the Hölder with the Hölder exponent 1, $u_0(x) = e^{-\lvert x\rvert}$	-0.9294	-1.056
$H^{3/4}$, the Hölder with the Hölder exponent 3/4, $u_0(x) = \lvert\sin(x)\rvert^{3/4}$	-0.815	-0.9262
$H^{1/2}$, the Hölder with the Hölder exponent 1/2, $u_0(x) = \lvert\sin(x)\rvert^{1/2}$	-0.6905	-0.7723
$H^{1/4}$, the Hölder with the Hölder exponent 1/4, $u_0(x) = \lvert\sin(x)\rvert^{1/4}$	-0.6138	-0.6653

We see that on the initial condition with high smoothness (first line in the table), the first order of Chernoff tangency corresponds to a decreasing error rate of about $1/n$, and the second order – a decreasing rate of about $1/n^2$. This is in accordance with the conjecture from [12] and theorem from [6].

As the smoothness is lost (second line in the table and below), theory from [6] stops working, and the experimental evidence is the following: the convergence speed gradually decreases and the advantages of the Chernoff function with the second order of Chernoff tangency gradually vanish. Let us present the results from the table graphically:

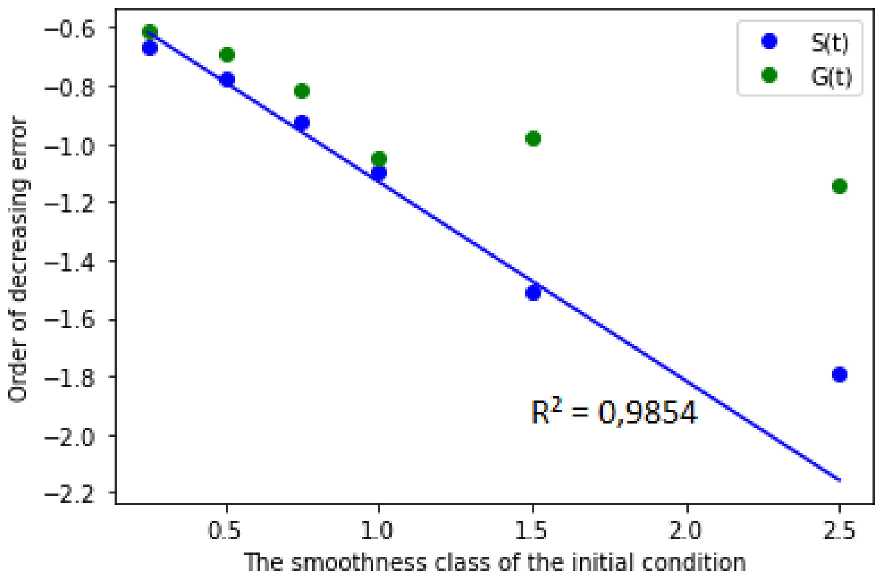


fig. 10

The regression was carried out without taking into account the point (2.5; 1.7923). The equation of the approximating line: $y = -0.684x - 0.4467$.This may be interpreted as follows: when the smoothness class α of the initial condition u_0 is not greater than the order of Chernoff tangency then

$$d = \|u_n(t,\cdot) - u(t,\cdot)\| = \sup_{x\in\mathbb{R}} |u_n(t,x) - u(t,x)| \approx \text{const} \cdot \left(\frac{1}{n}\right)^{0.68\alpha+0.45}.$$

Meanwhile when the smoothness class α of the initial condition u_0 is greater than the order of Chernoff tangency then there is no such easy-to-state dependence but still Chernoff function $S(t)$ with the second order Chernoff tangency provides better approximations than Chernoff function $G(t)$ with the first order Chernoff tangency.

Conclusion. The results of the numerical simulation are generally in agreement with and confirm the theory arising from the conjecture in [12]. However, some of the points that do not lie on straight lines exactly. This deserve closer attention: $n = 11$ for some initial conditions is not sufficient to derive conclusions about the asymptotic behavior of the calculation error. For not smooth initial conditions that we studied numerically there are not known any theoretical bounds on the rate of convergence. And, of course, the most interesting case of variable coefficients should be considered, understanding them as parameters analogously with u_0. So the research in this direction is far from ending.

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Appendix: Python 3 code

1.1 Moduli and variables

In [1]:
```
# importing moduli
import matplotlib.pyplot as plt
from sympy import oo
from scipy import integrate
import numpy as np
import math
```

In [2]:
```
# variables declaration
tau = 1/2
n = 11
```

In [3]:
```
l=[]
for i in range(1, n+1):
    l.append(math.log(i))
```

1.2 Functions and operators

```
# almost self-contained class
class classoffunctions(object):
    def thefunction(self, x):
        return x
```

```
# Chernoff function (S(t)f)(x)=(2/3)f(x) + (1/6)f(x + (6t)^(1/2)) + (1/6)f(x - (6t)^(1/2))
def oper(inputobject:classoffunctions, t):
    outputobject = inputobject
    f = inputobject.thefunction
    def funct(x):
        return (2/3)*f(x) + (1/6)*f(x + (6*t)**(1/2)) + (1/6)*f(x - (6*t)**(1/2))
    outputobject.thefunction = funct
    return outputobject
```

```
# Chernoff function (G(t)f)(x) = (1/4)* f(x+2t^(1/2))+(1/4) f(x-2t^(1/2))+(1/2)f(x)
def oper1(inputobject:classoffunctions, t):
    outputobject = inputobject
    f = inputobject.thefunction
    def funct(x):
        return (1/4)*f(x+2*t**(1/2))+(1/4)*f(x-2*t**(1/2))+(1/2)*f(x)
    outputobject.thefunction = funct
    return outputobject
```

```python
# composition degree of Chernoff function (S(t)f)(x)
def degr(g, tau, n):
    y = []
    obj = classoffunctions()
    for n_p in range(1, n + 1):
        obj_k = obj
        obj_k.thefunction = g
        for k in range(1, n_p + 1):
            obj_k = oper(obj_k, tau/n_p)
        y.append(obj_k.thefunction)
    return y
```

```python
# composition degree of Chernoff function (G(t)f)(x)
def degr1(g, tau, n):
    y = []
    obj = classoffunctions()
    for n_p in range(1, n + 1):
        obj_k = obj
        obj_k.thefunction = g
        for k in range(1, n_p + 1):
            obj_k = oper1(obj_k, tau/n_p)
        y.append(obj_k.thefunction)
    return y
```

```python
# norm computation
def norm(y, sol):
    d = []
    for n_p in range(0, n):
        d.append(np.max(np.abs(sol - y[n_p](x))))
    return d
```

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