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Solving probability transform functional equations for numerical inversion

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Many methods for numerically inverting transforms require values of the transform at complex arguments. However, in some applications, the transforms are only characterized implicitly via functional equations. This is illustrated by the busy-period distribution in the M/G/1 queue. In this paper we provide conditions for iterative methods to converge for complex arguments. Moreover, we show that stochastic monotonicity properties can provide useful bounds.

numerical transform inversion; Laplace transforms; functional equations; M/G/1 queue; busy period; implicitly defined transforms

1. Introduction and summary

In [1], [2] and [3] we describe effective methods for calculating probability cumulative distribution functions by numerically inverting transforms. These methods require values of the transform at selected (complex) arguments. In many applications this requirement is easily met, because an explicit expression for the transform is available. However, in some applications the transform is only characterized implicitly via a functional equation. In this paper we discuss ways to solve these functional equations to obtain the values of the transform required for the numerical inversion. In this paper we only discuss one-dimensional transforms, but similar methods apply to multidimensional transforms; see p. 35 of [1].

We were motivated by the busy-period distribution in the M/G/1 queue; e.g., see Section 6.8 of Cooper [6] or Section 1.2 of Neuts [14]. The busy-period distribution in turns plays an important role in the transient behavior of the M/G/1 queue (e.g., see Keilson and Kooharian [10], Section 1.3 of Takács [18], Ott [15], Chapter II.4 of Cohen [5] and Abate and Whitt [4]) and the steady-state behavior of M/G/1 models with priorities and other service disciplines (e.g., see Chapter III.3 of Cohen [5], Chapter 5 of Cooper [6], Doshi [7] and Neuts [14]).

We begin by describing this M/G/1 example. Let V be the cumulative distribution function (cdf) of a service time, which we assume has mean 1. Let

$$\hat{v}(s)=\int_0^{\infty} \mathrm{e}^{-st}\,\mathrm{d}V(t)=\int_0^{\infty}\mathrm{e}^{-st}v(t)\,\mathrm{d}t \qquad (1.1)$$

be the associated Laplace–Stieltjes transform (LST) of V and Laplace transform of its density v when $V(t)=\int_0^t v(u)\,\mathrm{d}u$ for all t. (All LSTs here are defined for complex numbers s with nonnegative real part Re(s).) Let the arrival rate of the Poisson arrival process (and the traffic intensity) be ρ where $0<\rho<1$. Let B be the cdf of a busy period and let

$$\hat{b}(s)=\int_0^{\infty} \mathrm{e}^{-st}\,\mathrm{d}B(t)=\int_0^{\infty}\mathrm{e}^{-st}b(t)\,\mathrm{d}t \qquad (1.2)$$

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be its LST and the Laplace transform of its density b when $B(t)=\int_0^t b(u)\,du$ for all t. The LST $\hat{b}$ is characterized by the Kendall functional equation

$$\hat{b}(s)=\hat{v}(s+\rho-\rho\hat{b}(s)); \tag{1.3}$$

see (8.67) on p. 230 of Cooper [6].

First, it is well known that (1.3) has a unique solution and that an analytical inversion is possible. In particular,

$$B(t)=\sum_{n=1}^{\infty}\int_0^t \frac{(\rho u)^{n-1}}{n!}e^{-\rho u}\,dV^{(n)}(u), \quad t\ge 0, \tag{1.4}$$

where $V^{(n)}$ is the n-fold convolution of V with itself; see (8.76) on p. 232 of Cooper [6]. However, in general (1.4) is not especially convenient for calculating $B(t)$, so that numerical inversion remains a viable alternative.

It is also well known that the functional equation (1.3) is easy to analyze when the variable s is a nonnegative real number. For any nonnegative real s, we can regard the right side as an operator T_s mapping the interval [0, 1] into itself, i.e.,

$$T_s(x)=\hat{v}(s+\rho-\rho x), \quad 0\le x\le 1. \tag{1.5}$$

It is easy to see that T_s is nondecreasing in x for all $\hat{v}$, with

$$T_s(0)=\hat{v}(s+\rho)>0 \text{ and } T_s(1)=\hat{v}(s)\le 1, \tag{1.6}$$

so that T_s has a unique fixed point in [0, 1] and (1.3) has a unique solution. Moreover, successive iterates of T_s converge monotonically to $b(s)$, i.e.,

$$T_s^n(x)\uparrow b(s) \text{ as } n\to\infty \quad \text{if } x<b(s) \tag{1.7}$$

and

$$T_s^n(x)\downarrow b(s) \text{ as } n\to\infty \quad \text{if } x>b(s); \tag{1.8}$$

see p. 232 of Cooper [6].

However, many numerical inversion procedures, including the principal ones in [1–3], require values of the transform for complex arguments s. For example, the algorithm EULER in [1,3] which implements a variant of the Fourier-series method for inverting Laplace transforms calculates a function value $f(t)$ via its Laplace transform

$$\hat{f}(s)=\int_0^{\infty}e^{-st}f(t)\,dt \tag{1.9}$$

by calculating weighted sum of the values of the real part of $\hat{f}(s)$ for s of the form $u+iv$ where $u\ge 0$; i.e., the numerical approximation is

$$f(t)\approx\sum_{k=0}^{n}a_k\,\mathrm{Re}(\hat{f})(u+ivk) \tag{1.10}$$

for appropriate positive integer n, positive real numbers u and v, and real numbers a_k.

Thus, with EULER, we would calculate the complementary busy-period cdf B^c, where $B^c(t)=1-B(t)$ for all t, by applying (1.10) with the Laplace transform

$$\hat{f}(s)=\hat{B}^c(s)\equiv\int_0^{\infty}e^{-st}B^c(t)\,dt=\frac{1-\hat{b}(s)}{s}. \tag{1.11}$$

Hence, to apply EULER to calculate $B^c(t)$, it suffices to determine $\hat{b}(s)$ for $s=u+iv$ for $u>0$ and $v>0$. The question is how to do this.

One approach is to avoid this difficulty by restricting attention to numerical inversion procedures that use only the transform values $\hat{f}(s)$ for real numbers s. For example, the Gaver [9]–Stehfest [16] procedure described in Section 8 of [1] has been used for this purpose by Gaver [9], Nance, Bhat and Claybrook [14], and Middleton [13]. This is a satisfactory approach, but as noted in [1], the Gaver–Stehfest procedure requires quite high precision to achieve good numerical accuracy.

What we would like to do to supply the transform values in (1.10) is simply iterate (1.5) for any desired complex s. When we tried it, we found that it worked. No doubt many others have discovered this as well; e.g., Bharat Doshi reports using this iterative scheme with complex arguments in [7]. Our first goal is to prove that this iterative scheme for the M/G/1 busy-period cdf does indeed always converge for all complex s. Unfortunately, however, we do not know how to give a *direct* proof that iteration of (1.5) always works for complex s as well as real s. We show that the iteration of (1.5) does in fact work for complex s by viewing the problem probabilistically.

It turns out that the idea of using a probabilistic argument to establish convergence of the iteration is not new. It appears in Theorem 3.1.5 of Lucantoni [11] and Sections 1.2 and 2.2 of Neuts [14]. They treat Markov chains of M/G/1 type, which includes the standard M/G/1 queue as a special case. However, they consider (1.5) only for the initial condition $x = 0$. In this context, our main contribution is to point out the significance of this reasoning for numerical transform inversion. We also consider more general initial conditions. We contribute further by showing that the monotonicity of the operator allows us to construct two-sided bounds on the final computation from approximations based on finitely many iterations (based on initial conditions $x = 0$ and $x = 1$). We also show how the procedure can be used more generally (outside the M/G/1 context).

Here is how the rest of this paper is organized. In Section 2 we establish the results for the M/G/1 busy period. In Section 3 we establish conditions for the procedure to work more generally. In Section 4 we give a numerical example for the M/G/1 busy period.

2. The M/G/1 busy period

We start by replacing (1.5) by an operator on Laplace transforms of possibly defective probability measures; i.e., we write

$$T(\hat{f}) \equiv T(\hat{f})(s) = \hat{v}(s + \rho - \rho \hat{f}(s)), \tag{2.1}$$

where s is a complex number with $\mathrm{Re}(s) \geq 0$ and $\hat{f}$ is the LST of a possibly defective cdf F, defined as in (1.1). Defective means that we allow $F(\infty) < 1$. For any fixed s, real or complex, we are just applying (1.5) with the stipulation that $x = \hat{f}(s)$ for some cdf F. For example, it suffices to let $x = 0$ or 1, because $\hat{f}(s) = 1$ for all s if $F(0) = 1$ and $\hat{f}(s) = 0$ for all s if $F(t) = 0$ for all t. However, for T to be a legitimate operator in this sense we must know that $T(\hat{f})$ itself is a LST of a possibly defective cdf.

Theorem 1. *If $\hat{f}$ is an LST of a possibly defective cdf F, then so is $T(\hat{f})$ for T in (2.1).*

Proof. We explicitly construct the cdf of which $T(\hat{f})$ is the LST. We use a probabilistic characterization of (1.3) often used in its proof; e.g., p. 229 of Cooper [6]. For this purpose, let S be a service time random variable, let $\{A(t): t \geq 0\}$ be a Poisson counting process with rate ρ and let X, X_1, $X_2, \ldots$ be i.i.d. random variables with the busy-period cdf. Then the probabilistic version of (1.3) is

$$X \stackrel{d}{=} S + \sum_{j=1}^{A(S)} X_j, \tag{2.2}$$

where $\stackrel{d}{=}$ denotes equality in distribution. Hence, we can express (2.1) equivalently as an operator T acting on (possibly defective) cdf's by

$$T(F) \equiv T(F)(t) = P\left(S + \sum_{j=1}^{A(S)} Y_j \leq t\right), \quad t \geq 0, \tag{2.3}$$

where S, $\{A(t): t \geq 0\}$ and $\{Y_j : j \geq 1\}$ are mutually independent, S has cdf V, $\{A(t): t \geq 0\}$ is a Poisson process with rate ρ and $\{Y_j,\ j \geq 1\}$ is a sequence of i.i.d. random variables with cdf F (having LST $\hat{f}$). Indeed, a direct calculation of the LST of (2.3) yields (2.1). □

We show that iterates of (1.5) converge as $n \to \infty$ for any complex s by showing that iterates of (2.1) converges as $n \to \infty$.

Theorem 2. *Let s be any complex number with $\mathrm{Re}(s) > 0$. If $x = \hat{f}(s)$ for some possibly defective cdf F, then $T_s^n(x) \to \hat{b}(s)$ as $n \to \infty$, where T_s is the operator in (1.5) and $\hat{b}$ is the unique solution to (1.3).*

Proof. By Theorem 1, $T^n(\hat{f})$ is an LST of a possibly defective cdf for all n; let F_n be the cdf associated with $T^n(\hat{f})$. For s real, the set of x such that $x = \hat{f}(s)$ for some cdf is the unit interval [0, 1]. As observed in Section 1, $T_s^n(x) \to \hat{b}(s)$ as $n \to \infty$ for all real s and all $x \in [0, 1]$. Hence, $T^n(\hat{f})(s) \to \hat{b}(s)$ for all real s, where T is the operator in (2.1). However, restricting attention to real s suffices to imply that the cdf's F_n converge to B as $n \to \infty$ in the sense that

$$F_n(t) \to B(t) \quad \text{as } n \to \infty \tag{2.4}$$

for all finite t that are continuity points of the limiting cdf $B(t)$; see p. 248 and Theorem 2a on p. 433 of Feller [8]. However, this convergence in turn implies that the transforms converge for all complex s with $\mathrm{Re}(s) > 0$. To see this, note that if $u > 0$, then $e^{-ut}\cos vt$ and $e^{-ut}\sin v(t)$ are continuous functions that vanish at infinity.

Hence, for each $s = u + iv$ with $u > 0$, the real and imaginary parts satisfy

$$\begin{aligned}\operatorname{Re} \hat{f}_n(s) &= \int_0^\infty \operatorname{Re} e^{-st}\, dF_n(t) = \int_0^\infty e^{-ut} \cos vt\, dF_n(t) \\ &\to \int_0^\infty e^{-ut} \cos vt\, dB(t) = \operatorname{Re} \hat{b}(s) \quad \text{as } n \to \infty,\end{aligned} \tag{2.5}$$

and

$$\begin{aligned}\operatorname{Im} \hat{f}_n(s) &= \int_0^\infty \operatorname{Im} e^{-st}\, dF_n(t) = \int_0^\infty e^{-ut} \sin vt\, dF_n(t) \\ &\to \int_0^\infty e^{-ut} \sin vt\, dB(t) = \operatorname{Im} \hat{b}(s) \quad \text{as } n \to \infty;\end{aligned} \tag{2.6}$$

see Theorem 1 on p. 249 of Feller [8]. Finally, existence and uniqueness of the solution to (1.3) for complex s are determined by the existence and uniqueness for real s. □

We remark that it is easy to see from the proof of Theorem 2 that the operator T in (2.1) is continuous using the mode of convergence in (2.4). We now show that the operator T is also monotone. As a consequence, we show that the iterates produce bounds on the busy period cdf if we start with appropriate initial transforms. For this purpose, we use the usual stochastic ordering. We say that one possibly defective cdf F_1 is *stochastically less than or equal to* another possibly defective cdf F_2, and write $F_1 \le_{st} F_2$, if $F_1(t) \ge F_2(t)$ for all t; e.g., see Stoyan [15].

Theorem 3. *If $F_1 \le_{st} F_2$, then $T(F_1) \le_{st} T(F_2)$, where $T(F_i)$ is the possibly defective cdf associated with $F_i(t) = P(Y_j^i \le t)$ in (2.3).*

Proof. From (2.3), it is immediate that $S + \sum_{j=1}^{A(S)} Y_j$ is increasing in $\{Y_j : j \ge 1\}$ for each realization of the random variables. If $F_1 \le_{st} F_2$, then it is possible to construct random variables $\{Y_j^i : j \ge 1\}$ such that $\{Y_j^i : j \ge 1\}$ is i.i.d., Y_1^i has cdf F_i and $Y_j^1 \le Y_j^2$ for all j w.p.1. Hence,

$$S + \sum_{j=1}^{A(S)} Y_j^1 \le S + \sum_{j=1}^{A(S)} Y_j^2 \quad \text{w.p. } 1$$

which implies that

$$T(F_1)(t) = P\left(S + \sum_{j=1}^{A(S)} Y_j^1 \le t\right) \ge P\left(S + \sum_{j=1}^{A(S)} Y_j^2 \le t\right) = T(F_2)(t)$$

for all t, so that indeed $T(F_1) \le_{st} T(F_2)$. □

In the space of (possibly defective) cdf's, the cdf's F_* and F^* with $F_*(t) = 1$ for all t and $F^*(t) = 0$ for all t are minimal and maximal elements, respectively, in the stochastic ordering; i.e., $F_* \le_{st} F \le_{st} F^*$ for all possibly defective cdf's F. The cdf's F_* and F^* correspond to a unit point mass at 0 and at infinity, respectively. The associated LSTs are $\hat{f}_*(s) = 1$ for all s and $\hat{f}^*(s) = 0$ for all s. If we use these extremal LSTs as starting points then we obtain bounds on the busy period cdf. The following is an easy consequence of Theorem 3.

Theorem 4. *The iterates $T_s^n(x)$ for $x = 1$ and $x = 0$ are LSTs $\hat{b}_{n*}(s)$ and $\hat{b}_n^*(s)$, respectively, of cdf's $B_{n*}(t)$ and $B_n^*(t)$ with*

$$\begin{aligned}1 &= f_*(s) \ge \hat{v}(s) = \hat{b}_{1*}(s) \ge \hat{b}_{n*}(s) \ge \hat{b}_{(n+1)_*}(s) \\ &\ge \hat{b}(s) \ge \hat{b}_{(n+1)}^*(s) \ge \hat{b}_n^*(s) \ge \hat{b}_1^*(s) \\ &= \hat{v}(s+\rho) \ge f^*(s) = 0\end{aligned} \tag{2.7}$$

for all n and positive real s, and

$$\begin{aligned}1 &= F_*(t) \ge V(t) = B_{1*}(t) \ge B_{n*}(t) \\ &\ge B_{(n+1)_*}(t) \ge B(t) \\ &\ge B_{n+1}^*(t) \ge B_n^*(t) \\ &\ge B_1^*(t) = P(S \le t,\ A(S) = 0) \ge F^*(t) = 0\end{aligned} \tag{2.8}$$

for all t and n.

As indicated in Section 1, results closely related to the theorems in this section appear in Theorem 3.1.5 of Lucantoni [11] and Sections 1.2 and 2.2 of Neuts [14]. They obtain one-sided bounds on the generalization of $B(t)$, paralleling (2.8). To make the connection, note that $P(S \le t, A(S) = k) = A_k(t)$ for $A_k(t)$ in (1.1.2) of [14] and $\hat{v}(s + \rho) = \tilde{A}_0(s)$ in (1.2.3) of [14]; i.e., the k-th iterate starting with $f^*(s) = 0$ corresponds to making the first passage in exactly k steps.

3. Other transform functional equations

We now indicate how the methods of Section 2 apply more generally. We suppose that we have a transform functional equation

$$\hat{f} = T(\hat{f}) \tag{3.1}$$

where $\hat{f}$ is the LST of a (possibly defective) cdf F.

Theorem 5. *Suppose that T in* (3.1) *is an operator mapping LSTs of possibly defective cdf's into LSTs of possibly defective cdf's. If $T^n(\hat{g})(s) \to \hat{f}(s)$ as $n \to \infty$ for some LST $\hat{g}$ of a possibly defective cdf and all real s, then*

$$F_n(t) \to F(t) \quad \text{as} \quad n \to \infty \tag{3.2}$$

for all t that are continuity points of F, where $F_n(t)$ is the possibly defective cdf with LST $T^n(\hat{g})$ and $F(t)$ is the possibly defective cdf with LST $\hat{f}$. Moreover, if (3.2) *holds, then $T^n(\hat{g})(s) \to \hat{f}(s)$ as $n \to \infty$ for all complex s with* $\mathrm{Re}(s) > 0$.

Proof. Apply the argument used to prove Theorem 2. □

We now give a sufficient condition for the convergence condition in Theorem 5.

Theorem 6. *Suppose that the operator T in* (3.1) *can be represented by*

$$T(\hat{f})(s) = T_s(\hat{f}(s)) \tag{3.3}$$

for each real number s, where T_s is nondecreasing real-valued function for a real variable with $T_s(0) > 0$ and $T_s(1) \le 1$ for each positive real s. Then $T_s^n(x) \to \hat{f}(s)$ as $n \to \infty$ for each positive real s and each x with $0 \le x \le 1$.

Proof. Apply the argument in (1.5)–(1.8). □

Combining Theorems 5 and 6 we also obtain Laplace transform stochastic orderings generalizing (2.7); see p. 22 of Stoyan [17].

Theorem 7. *Under the conditions of both Theorems 5 and 6,*

$$\begin{aligned} 1 = \hat{f}_*(s) &\ge T^n(\hat{f}_*)(s) \ge T^{n+1}(\hat{f}_*)(s) \ge \hat{f}(s) \\ &\ge T^{n+1}(\hat{f}^*)(s) \ge T^n(\hat{f}^*)(s) \ge \hat{f}^*(s) = 0 \end{aligned} \tag{3.4}$$

for all n and real positive s.

In doing a numerical inversion we may work with complex s and have convergence of successive iterates of the operator T in (3.1) by virtue of Theorem 5. Theorem 7 tells us that in the case of (3.3) the cdf's associated with those iterations are ordered in the Laplace transform ordering in (3.4) involving all positive real s. The Laplace transform ordering in turn implies that the moments are ordered in a certain way. However, (3.4) is not so useful to check calculations, because for the numerical inversions using (1.10) iterations of (3.3) are only done for finitely many complex s and the numerical inversion produces only the cdf values $F_{n*}(t)$ and $F_n^*(t)$ for finitely many t. We thus do not directly produce the transform values in (3.4). However, we could do the iterations of (3.3) also for several real s to get an idea about the quality of the approximations. From Theorem 7, we see that $T^n(\hat{f}_*)(s) - T^n(\hat{f}^*)(s)$ for real s is an upper bound on the error in the calculation of $\hat{f}(s)$ after n iterations.

However, under extra conditions, we get useful direct bounds on the cdf. Theorem 3 shows that these conditions hold for the M/G/1 busy period.

Table 1
Successive iterates of operator (2.1) in the M/G/1 example in Section 4 with $s = 0.3979167 + 0.6544985i$.

iteration	real part	imaginary part	modulus
starting with $\hat{b}_0(s) = 0$			
1	0.5215651	−0.0997833	0.5310244
2	0.5664467	−0.1524585	0.5866050
3	0.5652960	−0.1629180	0.5883042
4	0.5639880	−0.1638444	0.5873052
5	0.5639511	−0.1637884	0.5870621
6	0.5637337	−0.1637559	0.5870364
7	0.5637357	−0.1637506	0.5870368
8	0.5637365	−0.1637503	0.5870374
9	0.5637366	−0.1637504	0.5870376
starting with $\hat{b}_0(s) = 1$			
1	0.6378206	−0.2077858	0.6708130
2	0.5657992	−0.1768587	0.5927966
3	0.5624473	−0.1652914	0.5862322
4	0.5634320	−0.1637582	0.5867473
5	0.5637051	−0.1637165	0.5869979
6	0.5637373	−0.1637434	0.5870363
7	0.5637374	−0.1637497	0.5870382
8	0.5637367	−0.1637504	0.5870377
9	0.5637366	−0.1637504	0.5870376

Table 2
Numerical estimates of the M/G/1 busy-period complementary cdf $B^c(t)$ for the example in Section 4 as a function of the number of iterations of (2.1). Each displayed value is (estimate-exact)$\times 10^6$, with no number meaning less than 0.5 and '×' meaning greater than 100

time	exact values	initial condition $\hat{b}_0(s)=1$			initial condition $\hat{b}_0(s)=0$		
		number of iterations			number of iterations		
		10	20	30	10	20	30
0.5	0.518004						
1	0.392419						
2	0.274266						
6	0.132691						
12	0.074877	−1			1		
24	0.037027	−×			×		
48	0.014822	−×			×		
96	0.004138	−×	−14		×	26	
192	0.000606	−×	−60	−1	×	×	2
288	0.000119	−×	−×	−3	×	×	14

Theorem 8. *Suppose that T in* (3.1) *is an operator mapping LSTs of possibly defective cdf's into LSTs of possibly defective cdf's. Moreover, suppose that T regarded as an operator mapping possibly defective cdf's into possibly defective cdf's is monotone in the stochastic ordering. Then*

$$1 = F_*(t) \geq F_{n*}(t) \geq F_{(n+1)*}(t) \geq F(t)$$
$$\geq F_{n+1}^*(t) \geq F_n^*(t) \geq F^*(t) = 0$$

for all t and n, where F_{n*} and F_n^* are the cdf's associated with $T^n(\hat{f}_*)$ and $T^n(\hat{f}^*)$, respectively.

4. A numerical example

We conclude by reporting a numerical example. In particular, we apply the algorithms EULER and POST-WIDDER for inverting Laplace transforms in [1] and [3] plus iteration of (2.1) to compute the complementary busy-period cdf $B^c(t)$ for the M/G/1 queue when the service-time distribution has a gamma distribution with mean 1 and shape parameter $\frac{1}{2}$ and the arrival rate is $\rho = 0.75$. Thus, the service-time LST is $\hat{v}(s) = (1+2s)^{-1/2}$.

Table 1 displays successive iterates of (2.1) starting with $\hat{b}_0(s) = f_*(s) = 1$ and $\hat{b}_0(s) = \hat{f}^*(s) = 0$ when $s = 0.3979167 + 0.6544985i$. We display the real part, $\text{Re}[T^n(b_0(s))]$, the imaginary part, $\text{Im}[T^n(b_0(s))]$, and the modulus, $(\text{Re}[T^n(b_0(s))]^2 + \text{Im}[T^n(b_0(s))]^2)^{1/2}$. From Table 1, we see evidence of convergence, but no monotonicity. Moreover, the absolute values of the increments are not monotone, so that there is not a contraction property associated with these terms. (Recall that we have no positive results other than convergence for the successive iterates of the *transforms* for complex numbers s.)

Table 2 displays the numerical estimates of the complementary cdf $B^c(t)$ for several different values of t based on 10, 20 and 30 iterations. Using the two inversion algorithms EULER and POST-WIDDER confirmed accuracy to 10^{-8} in the inversion, so that the reported errors are due solely to the iteration of (2.1). The monotonicity in n from above and below is evident from the results. Moreover, we see that more iterations are required for higher values of t. However, satisfactory guaranteed accuracy is consistently achieved with a modest computation.

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