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The logistic-normal integral and its generalizations

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ABSTRACT

We consider the solutions of the one-dimensional heat equation in an unbounded domain with initial conditions of the form $f(x)/(1+\exp(\sigma x))$. This includes as a particular case the logistic-normal integral, which corresponds to $f(x)=1$. Such initial conditions appear in stochastic calculus problems, and the numerical simulation of short-rate interest rate models and credit models with log-normally distributed short rates and hazard rates respectively. We show that the solutions at time t can be computed exactly on a grid of equidistant points of width σt in terms of the solutions of the heat equation with initial condition $f(x)$. The exact results on the grid can be used as nodes for a precise interpolation. Series representation of the solutions can be obtained by an application of the Poisson summation formula.

1. Introduction

The initial-value problem for the one-dimensional heat equation on $\mathbb{R}\times(0,\infty)$

$$\partial_t\varphi(z,t)=\frac{1}{2}\partial_z^2\varphi(z,t) \tag{1}$$

$$\varphi(z,0)=g(z) \tag{2}$$

has a unique solution in the space of infinitely differentiable functions $\varphi\in C^\infty(\mathbb{R}\times(0,\infty))$, provided that the initial condition $g(z)$ is continuous and essentially bounded $g\in C(\mathbb{R})\cap L^\infty(\mathbb{R})$ [1]. This equation is solved in terms of a convolution integral of the initial condition with the fundamental solution of the heat equation

$$\varphi(z,t)=\int_{-\infty}^{\infty}\frac{dx}{\sqrt{2\pi t}}e^{-\frac{1}{2t}(x-z)^2}g(x). \tag{3}$$

In general, the evaluation of this integral for arbitrary initial conditions $g(x)$ cannot be performed in closed form, and various approximation methods have to be applied.

We consider in this note the class of integrals of the form

$$\varphi(z,\sigma,t)=\int_{-\infty}^{\infty}\frac{dx}{\sqrt{2\pi t}}\frac{e^{-\frac{1}{2t}(x-z)^2}}{1+e^{\sigma x}}f(x) \tag{4}$$

with $t>0$, σ a real number, and $f(x)$ an arbitrary bounded function $f\in L^\infty(\mathbb{R})$. The case $f(x)=1$ corresponds to the so-called logistic-normal integral, which appears in statistics in problems of logistic regression [2]. To our knowledge no closed form result for this integral is known. Various approximations have been proposed in the literature, which are summarized

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in Chapter 7.1.2 of [3], see also Section 18.4 of [2], and [4]. A precise numerical evaluation of the logistic-normal integral was given in [5] using trapezoidal quadrature with step h

$$\varphi(z,\sigma,t)=h\sum_{k=-\infty}^{\infty}\frac{1}{\sqrt{2\pi t}}e^{-\frac{1}{2t}(z-hk)^2}\frac{1}{1+e^{\sigma hk}}+E(h). \tag{5}$$

The approximation error $E(h)$ can be controlled using a method proposed in [6], and is bounded as [5]

$$|E(h)|\le\begin{cases}2\exp\left(-\dfrac{2\pi^2 t}{h^2}\right), & \sigma\le\dfrac{h}{4t}\\ 2\exp\left(\dfrac{\pi^2}{8\sigma^2 t}-\dfrac{\pi^2}{\sigma h}\right), & \sigma>\dfrac{h}{4t}.\end{cases} \tag{6}$$

The method of [6] for bounding the integration error can be applied also to the case of an arbitrary $f(x)$, but it requires knowledge about the analytical structure of this function, and cannot be used if $f(x)$ is only known in numerical form.

Integrals of the form (4) appear also in the numerical simulation of short rate models with log-normally distributed short rates, such as the Black, Derman, Toy (BDT) or the Black, Karasinski (BK) models with a continuous state variable [7,8]. The calibration of these models is performed using a forward recursion for the Arrow–Debreu function [9], which requires the calculation of integrals of the form (4). Finally, the same integrals appear in the calibration of single-name credit models with log-normally distributed hazard rates [10]. A precise and fast method for the calculation of these integrals is clearly of interest for many practical applications.

We prove several exact results for the class of integrals (4), and show that their values can be found in closed form on a grid of equidistant points of width σt, provided that the simpler integrals

$$f(z,t)=\int_{-\infty}^{\infty}\frac{dx}{\sqrt{2\pi t}}e^{-\frac{1}{2t}(x-z)^2}f(x) \tag{7}$$

can be obtained in closed form. For $\sigma t\ll 1$ the equidistant points form a dense grid, which can be used as nodes for a very precise interpolation of $\varphi(z,\sigma,t)$. These results follow from recurrence relations satisfied by the functions $\varphi(z,\sigma,t)$ which determine them everywhere in terms of their values within one quasi-period of width σt.

We derive the recurrence relations in Section 2, and apply them to the simplest integral of type (4) corresponding to $f(x)=1$ (the logistic-normal integral) in Section 3. In Section 4 we consider the most general class of integrals of type (4). In Section 5 we present the application of this method to a few simple examples, and give an estimate for the interpolation error from the exact grid values. In Section 6 we present a method for obtaining series expansions for the integrals (4) using the Poisson summation formula, and illustrate it on the example of the logistic-normal integral.

2. Recurrence relations

The results of this note follow from the following simple observation. Assume that the functions $g_i(x)$ and $f_i(x)$ are related as

$$g_i(x)=\sum_{j=1}^{n}a_{ij}e^{b_{ij}x}g_j(x)+f_i(x) \tag{8}$$

with $a_{ij}, b_{ij}\in\mathbb{R}$. Then the solutions of the heat equation with initial conditions $g_i(x), f_i(x)$ are related by recurrence relations

$$\varphi_i(z,t)=\sum_{j=1}^{n}a_{ij}e^{b_{ij}z+\frac{1}{2}b_{ij}^2 t}\varphi_j(z+b_{ij}t,t)+f_i(z,t) \tag{9}$$

where $f_i(z,t)$ are defined as

$$f_i(z,t)=\int_{-\infty}^{\infty}\frac{dx}{\sqrt{2\pi t}}e^{-\frac{1}{2t}(x-z)^2}f_i(x). \tag{10}$$

Under certain conditions, the latter solutions can be found in closed form. This is the case for a wide class of functions $f(x)$, such as polynomials and certain trigonometric functions. Then the relation (9) can be used to obtain information about the solution $\varphi(z,t)$, and in some cases to find exact results for this solution.

As an application of this observation we consider in this note the class of integrals defined in (4). The argument above shows that the functions $\varphi(z,\sigma,t)$ satisfy the recurrence relations

$$\varphi(z+\sigma t,\sigma,t)=e^{-\sigma z-\frac{1}{2}\sigma^2 t}(f(z,t)-\varphi(z,\sigma,t)). \tag{11}$$

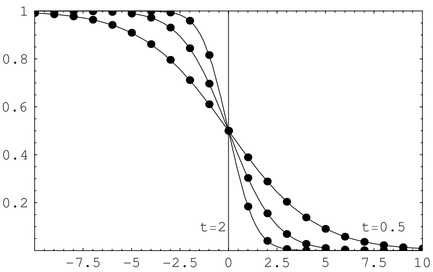

Fig. 1. Numerical result for the logistic-normal integral $\varphi(z/t, t)$ (solid lines) and the exact results (dots) obtained using (20), for $t = 0.5, 1, 2$.

This follows directly from (9) by noting that we have

$$\frac{f(x)}{1+e^{\sigma x}} = -e^{\sigma x}\frac{f(x)}{1+e^{\sigma x}} + f(x) \tag{12}$$

which has the form of Eq. (8) with $a = -1$, $b = \sigma$.

The recurrence relations (11) have a few interesting implications. First, assuming that $f(z, t)$ is known, the relation (11) allows the computation of $\varphi(z, \sigma, t)$ on a grid of equidistant points of width $z_0 + k\sigma t$, provided that it is computed at one particular point z_0.

A related result is

Remark 1. Assuming that $f(z, t)$ is known in closed form, knowledge of $\varphi(z, \sigma, t)$ in an interval of the form $(z_0, z_0 + \sigma t)$ is sufficient to obtain the values of this function for any $z \in \mathbb{R}$ by repeated application of Eq. (11).

This simplifies very much the numerical evaluation of $\varphi(z, \sigma, t)$, as it is sufficient to obtain the values of this function within an arbitrary quasi-period of width σt.

3. The logistic-normal integral

As a first application of these results, consider the simplest integral of type (4), corresponding to $f(z) = 1$. This is called the logistic-normal integral and is defined as

$$I(z; \sigma, t) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi t}} e^{-\frac{1}{2t}(x-z)^2} \frac{1}{1+e^{\sigma x}}. \tag{13}$$

This integral satisfies the rescaling relation

$$I(z; \sigma, t) = I\left(\frac{z}{\lambda}; \lambda\sigma, \frac{t}{\lambda^2}\right), \tag{14}$$

which means that it depends only on two combinations of the three parameters z, t, σ. We will choose $\sigma = 1$, and define the function $\varphi(z, t) \equiv I(z; 1, t)$, in terms of which the most general integral $I(z; \sigma, t)$ is written as

$$I(z; \sigma, t) = \varphi(\sigma z, \sigma^2 t). \tag{15}$$

The integral $\varphi(z, t)$ satisfies the recurrence relation following from Eq. (11)

$$\varphi(z + t, t) = e^{-z-\frac{1}{2}t}(1 - \varphi(z, t)). \tag{16}$$

This relation expresses a quasi-periodicity condition[1] for the function $\varphi(z, t)$. It states that knowledge of this function within a quasi-period $(z_0, z_0 + t)$ allows its determination for any other value of z by repeated application of (16). This property is somewhat surprising, as the shape of the function $\varphi(z, t)$ does not display any obvious periodicity, see Fig. 1.

The values of $\varphi(z, t)$ for positive and negative arguments are related as

$$\varphi(z, t) + \varphi(-z, t) = 1. \tag{17}$$

This can be derived by substituting here the definition (13), which gives upon changing variable $x \to -x$ in the second integral

$$\varphi(z, t) + \varphi(-z, t) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi t}} e^{-\frac{1}{2t}(x-z)^2} \left(\frac{1}{1+e^{\sigma x}} + \frac{1}{1+e^{-\sigma x}}\right) = 1. \tag{18}$$

[1] The function $\varphi(z, t)$ is also quasi-periodic along the imaginary axis with quasi-period $2\pi i$. Applying the Cauchy formula to the integral for $\varphi(z, t)$ taken along a rectangular contour with vertices at $\pm\infty$ and $\pm\infty - 2\pi i$ it is easy to check that it satisfies the relation $\varphi(z + 2\pi i, t) = \varphi(z, t) - i\sqrt{2\pi/t}\exp(-\frac{1}{2\pi}(z + i\pi)^2)$.

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Table 1
The first few values of the logistic-normal integral $\varphi(z_k, t)$ following from Eq. (20).

k	$\varphi(z_k, t)$
0	$\frac{1}{2}$
1	$\frac{1}{2}e^{-\frac{1}{2}t}$
2	$-\frac{1}{2}e^{-2t} + e^{-\frac{3}{2}t}$
3	$\frac{1}{2}e^{-\frac{9}{2}t} - e^{-4t} + e^{-\frac{5}{2}t}$
4	$-\frac{1}{2}e^{-8t} + e^{-\frac{15}{2}t} - e^{-6t} + e^{-\frac{7}{2}t}$
5	$\frac{1}{2}e^{-\frac{25}{2}t} - e^{-12t} + e^{-\frac{21}{2}t} - e^{-8t} + e^{-\frac{9}{2}t}$

From Eq. (17) one can obtain the value of the integral at $z = 0$

$$\varphi(0, t) = \frac{1}{2}. \tag{19}$$

This can be used as a starting point for the recurrence relation (16) to derive the values of $\varphi(z, t)$ at all points $z_k = kt$, with $k \in \mathbb{Z}$. These values can be written in compact form as

$$\varphi(z_{k+1}, t) = \sum_{j=1}^{k} (-)^{j+1} e^{\left(\frac{1}{2}j^2 - (k+1)j\right)t} + (-)^k \frac{1}{2} e^{-\frac{1}{2}(k+1)^2 t} \tag{20}$$

for all $k \geq 1$. The values of $\varphi(z_k, t)$ for negative z_k are related to those for positive z_k by Eq. (17). The first few values of $\varphi(z_k, t)$ are given in the Table 1. We show in Fig. 1 plots of the integral $\varphi(z, t)$ obtained by numerical integration, comparing them with the exact results from (20). These exact results for $\varphi(z, t)$ can be used as nodes for a precise interpolation of this function, using for example spline interpolation or cardinal series. The latter approach is discussed in detail in Section 5.

The function $\varphi(z, t)$ of complex argument is bounded as $|\varphi(x + iy, t)| \leq \exp(y^2/(2t))$, which implies that is has no poles for finite $|z|$. On the real axis it is bounded from above and below as

$$\frac{1}{1 + e^{z + \frac{1}{2}t}} \leq \varphi(z, t) \leq \frac{1}{1 + e^{z - \frac{1}{2}t}}. \tag{21}$$

The lower bound follows from the Jensen inequality, and the upper bound follows from the lower bound after using the relation (17).

4. A wider class of initial conditions

The methods used in the previous section can be applied for a wider class of initial conditions for the heat equation. Consider the integrals of the form

$$\varphi^{(\pm)}(z, \sigma, t) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi t}} \frac{e^{-\frac{1}{2t}(x-z)^2}}{1 + e^{\sigma x}} f^{(\pm)}(x) \tag{22}$$

where $f^{(\pm)}(x)$ is a even (odd) function of x

$$f^{(\pm)}(-x) = \pm f^{(\pm)}(x). \tag{23}$$

This is a generalization of the logistic-normal integral $\varphi(z, t)$ considered in the previous section, which corresponds to $f(x) = 1$.

Define also the simpler integral

$$f^{(\pm)}(z, t) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi t}} e^{-\frac{1}{2t}(x-z)^2} f^{(\pm)}(x). \tag{24}$$

This can be found in closed form for a wide class of functions $f^{(\pm)}(x)$, such as polynomials, certain trigonometric functions, etc.

The functions $\varphi^{(\pm)}(z, \sigma, t)$ satisfy the recurrence relations (11)

$$\varphi^{(\pm)}(z + \sigma t, \sigma, t) = e^{-\sigma z - \frac{1}{2}\sigma^2 t}(f^{(\pm)}(z, t) - \varphi^{(\pm)}(z, \sigma, t)). \tag{25}$$

We would like to find values of $\varphi^{(\pm)}(z, \sigma, t)$ at particular points, which can be used as starting points for the recurrence relation (25) in order to determine their values on a grid of equidistant points with width σt. This could be done for example by numerical evaluation of these functions at particular points. However, there are certain special points where $\varphi^{(\pm)}(z, \sigma, t)$ can be found exactly, as we show next. We consider separately the cases of even and odd $f^{(\pm)}(z)$.

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Even $f(x)$ case. The function $f^{(+)}(z,t)$ is even in z, $\varphi^{(+)}(z,\sigma,t)-\frac{1}{2}f^{(+)}(z,t)$ is odd in z. This can be seen by writing this difference as

$$\varphi^{(+)}(z,\sigma,t)-\frac{1}{2}f^{(+)}(z,t) = \int_{-\infty}^{\infty}\frac{dx}{\sqrt{2\pi t}}e^{-\frac{1}{2t}(x-z)^2}f^{(+)}(x)\left(\frac{1}{1+e^{\sigma x}}-\frac{1}{2}\right)$$
$$= -\frac{1}{2}\int_{-\infty}^{\infty}\frac{dx}{\sqrt{2\pi t}}e^{-\frac{1}{2t}(x-z)^2}f^{(+)}(x)\tanh\left(\frac{\sigma x}{2}\right), \tag{26}$$

which gives the solution of the heat equation with an initial condition odd in x. This is also an odd function of z, and thus it vanishes at $z=0$. This implies that the value of $\varphi^{(+)}(0,\sigma,t)$ is simply determined in terms of $f^{(+)}(0,t)$ as

$$\varphi^{(+)}(0,\sigma,t)=\frac{1}{2}f^{(+)}(0,t). \tag{27}$$

In conclusion, knowledge of $f^{(+)}(k\sigma t,t)$ with $k\in\mathbb{Z}$ allows the determination of $\varphi^{(+)}(k\sigma t,\sigma,t)$ by repeated application of the recursion relation (25) starting with the value of $\varphi^{(+)}(0,\sigma,t)$ given in (27).

Odd $f(x)$ case. The function $f^{(-)}(z,t)$ is odd in z. In contrast with the previous case, the value of $\varphi^{(-)}(0,\sigma,t)$ cannot be simply determined in terms of $f^{(-)}(0,t)$. The same argument as before gives instead a nonvanishing result

$$\varphi^{(-)}(0,\sigma,t)=-\frac{1}{2}\int_{-\infty}^{\infty}\frac{dx}{\sqrt{2\pi t}}e^{-\frac{1}{2t}x^2}\tanh\left(\frac{\sigma x}{2}\right)f^{(-)}(x). \tag{28}$$

If the integral (28) could be evaluated in some way, this would supply the initial value for the recursion, which would give $\varphi^{(-)}(k\sigma t,\sigma,t)$ at all points $z_k=k\sigma t$. We show next that such an initial value can be found on the grid of half-integer multiples of σt, as $\varphi^{(-)}(\frac{1}{2}\sigma t,\sigma,t)=0$.

It is convenient to represent the functions $\varphi^{(\pm)}(z,\sigma,t)$ in terms of new functions $g^{(\pm)}(z,\sigma,t)$ defined as

$$\varphi^{(\pm)}(z,\sigma,t)=e^{-\frac{1}{2}\sigma z}g^{(\pm)}\left(z-\frac{1}{2}\sigma t,\sigma,t\right), \tag{29}$$

where $g^{(\pm)}(z,\sigma,t)$ are related to the solutions of the heat equation with the initial condition $f^{(\pm)}(x)/\cosh(\sigma x/2)$

$$g^{(\pm)}(z,\sigma,t)=e^{\frac{1}{8}\sigma^2 t}\int_{-\infty}^{\infty}\frac{dx}{\sqrt{2\pi t}}e^{-\frac{1}{2t}(x-z)^2}\frac{f^{(\pm)}(x)}{2\cosh\frac{\sigma x}{2}}. \tag{30}$$

Since $f(x)$ was assumed to be bounded $f\in L^\infty$, the new initial condition for the heat equation $\frac{f^{(\pm)}(x)}{\cosh(\sigma x/2)}$ is integrable. This implies that $g(z,\sigma,t)$ will be also integrable $g\in L^1$. (Note that $\varphi^{(\pm)}(z,\sigma,t)$ are not in general integrable.)

The functions $g^{(\pm)}(z,\sigma,t)$ satisfy the difference equation

$$e^{-\frac{1}{2}\sigma z}g^{(\pm)}\left(z-\frac{1}{2}\sigma t,\sigma,t\right)+e^{\frac{1}{2}\sigma z}g^{(\pm)}\left(z+\frac{1}{2}\sigma t,\sigma,t\right)=f^{(\pm)}(z,t), \tag{31}$$

which follows from the recurrence relation (25). This relation will be used below in Section 6.

The functions $g^{(\pm)}(z,\sigma,t)$ are even/odd functions of z

$$g^{(\pm)}(-z,\sigma,t)=\pm g^{(\pm)}(z,\sigma,t). \tag{32}$$

In particular, the function $g^{(-)}(z,\sigma,t)$ vanishes at $z=0$, which gives

$$\varphi^{(-)}\left(\frac{1}{2}\sigma t,\sigma,t\right)=0. \tag{33}$$

This can be used as initial value for the recursion relation (25), which determines thus the function $\varphi^{(-)}(z_k,\sigma,t)$ at all values of $z_k=(k+\frac{1}{2})\sigma t$ equal to half-integers of σt.

In conclusion, we have proven the following theorem concerning the functions $\varphi^{(\pm)}(z,\sigma,t)$ defined in Eq. (22).

Theorem 1. *The functions $\varphi^{(\pm)}(z,\sigma,t)$ satisfy the recurrence relations (25). They can be used to determine the values of these functions on grids of equidistant points, defined as follows.*

- *Even $f(x)$ functions: one can find $\varphi^{(+)}(z_k=k\sigma t,\sigma,t)$ at all values of z equal to integer multiples of σt, starting with $\varphi^{(+)}(0,\sigma,t)=\frac{1}{2}f(0,t)$.*
- *Odd $f(x)$ functions: one can find $\varphi^{(-)}(z_k=(k+\frac{1}{2})\sigma t,t)$ at all values of z equal to half-integer multiples of σt, starting with $\varphi^{(-)}(\frac{1}{2}\sigma t,\sigma,t)=0$.*

This is the main result of this paper.

The method of the recurrence relations can be applied also if the constants a_{ij} and b_{ij} in Eq. (8) are piece-wise constant functions. In particular this holds for initial conditions of the form $f(x)/(1+e^{\sigma(x)x})$ with $\sigma(x)$ a piece-wise constant function of x. Splitting the integration over x into pieces corresponding to regions where $\sigma(x)$ is a constant, each of the resulting integrals over x regions satisfies recurrence relations of the same type as their sum, and the Theorem 1 can be used to obtain information about this integral, as we explain next.

Denote $D \in \mathbb{R}$ a region of the real axis where $\sigma(x)$ takes a constant value σ_D. The region D can be either finite (a, b) or semi-infinite, of the form $(-\infty, b)$ or (a, ∞). For definiteness we will denote D in the following as a finite interval (a, b). Then the integral

$$\varphi_D(z,t) = \int_a^b \frac{dx}{\sqrt{2\pi t}} e^{-\frac{1}{2t}(x-z)^2} \frac{f(x)}{1+e^{\sigma_D x}} \tag{34}$$

satisfies the recurrence relation

$$\varphi_D(z+\sigma_D t, t) = e^{-\sigma_D z - \frac{1}{2}\sigma_D^2 t}(f(z,t) - \varphi_D(z,t)), \tag{35}$$

where $f(z, t)$ is defined as

$$f(z,t) = \int_a^b \frac{dx}{\sqrt{2\pi t}} e^{-\frac{1}{2t}(x-z)^2} f(x). \tag{36}$$

These integrals can be extended to the entire real axis by defining the function $\bar{f}(x)$ as

$$\bar{f}(x) = \begin{cases} f(x), & x \in D \\ 0, & x \in \mathbb{R} \setminus D. \end{cases} \tag{37}$$

The integral $\varphi_D(z, t)$ can be written as a sum of two integrals $\varphi_D(z,t) = \varphi_D^{(+)}(z,t) + \varphi_D^{(-)}(z,t)$, corresponding to the decomposition of $\bar{f}(x)$ into its even and odd components

$$\varphi_D^{(\pm)}(z,t) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi t}} e^{-\frac{1}{2t}(x-z)^2} \frac{\bar{f}^{(\pm)}(x)}{1+e^{\sigma_D x}} \tag{38}$$

$$\bar{f}^{(\pm)}(x) = \frac{1}{2}(\bar{f}(x) \pm \bar{f}(-x)). \tag{39}$$

The support of $\bar{f}^{(\pm)}(x)$ is $D \cup \bar{D}$, where $\bar{D}$ is the mirror reflection of D around the origin. Thus the integral over x in Eq. (38) actually runs only over $x \in D \cup \bar{D}$. Now the Theorem 1 can be directly applied: both $\varphi_D^{(\pm)}(z,t)$ satisfy the recurrence relations (35), and one can find $\varphi_D^{(+)}(z_k = k\sigma_D t, t)$ on the grid of integer multiples of $\sigma_D t$ and $\varphi_D^{(-)}(z_k = (k+\frac{1}{2})\sigma_D t, t)$ on the grid of half-integer multiples of $\sigma_D t$, with $k \in \mathbb{Z}$, starting with the initial conditions

$$\varphi_D^{(+)}(0,t) = \frac{1}{2}\bar{f}^{(+)}(0,t), \qquad \varphi_D^{(-)}\left(\frac{1}{2}\sigma_D t, t\right) = 0, \tag{40}$$

provided that $\bar{f}^{(\pm)}(z, t)$ are known in closed form.

5. Examples and an error estimate

We illustrate in this section the general method presented in the previous section on the example of the integrals of the form

$$\varphi_j(z,t) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi t}} e^{-\frac{1}{2t}(x-z)^2} \frac{x^j}{1+e^x}. \tag{41}$$

The corresponding simpler functions

$$f_j(z,t) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi t}} e^{-\frac{1}{2t}(x-z)^2} x^j = (-t)^{j/2} H_j\left(\frac{x}{\sqrt{-t}}\right) \tag{42}$$

can be expressed in terms of Hermite polynomials, and are known as the heat polynomials [11]. The first few functions $f_j(x, t)$ are

$$f_0(x,t) = 1 \tag{43}$$

$$f_1(x,t) = x \tag{44}$$

$$f_2(x,t) = x^2 + t \tag{45}$$

$$f_3(x,t) = x^3 + 3xt. \tag{46}$$

We used here the probabilists' Hermite polynomials, defined as $H_j(x) = (-)^j \exp(x^2/2)\partial_x^j \exp(-x^2/2)$.

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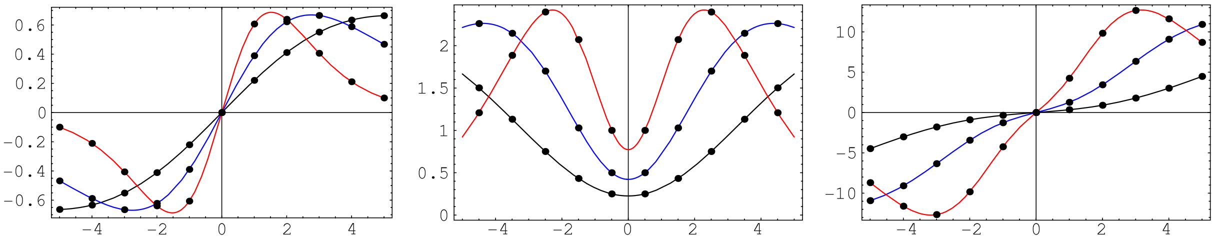

Fig. 2. The functions $g_j(z/t, t)$ for $j = 1, 2, 3$ and $t = 0.5$ (black), $t = 1$ (blue) and $t = 2$ (red). The dots show the exact values obtained as explained in the text, and the solid curves show the results of numerical integration. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

According to the general method presented in the previous section, we treat the cases of even and odd j separately. The even-index functions $\varphi_{2j}(z)$ can be found exactly at $z = kt$, while the odd-index functions $\varphi_{2j+1}(z)$ can be found exactly at $z = (k + \frac{1}{2})t$. This can be done using the recursion relation (11), starting with the initial values

$$\varphi_{2j}(0, t) = \frac{1}{2} f_{2j}(0, t) = \frac{(2j)!}{2j!} \left(\frac{t}{2}\right)^j, \qquad \varphi_{2j+1}\left(\frac{1}{2}t, t\right) = 0. \tag{47}$$

In practice it is easier to compute the functions $g_j(z, t)$ which are defined as in (30) and are related to $\varphi_j(z, t)$ as

$$\varphi_j(z, t) = e^{-z/2} g_j\left(z - \frac{1}{2}t, t\right). \tag{48}$$

Since $g_j(z, t)$ are even (for even index j), and odd (for odd index j), it is sufficient to compute their values by recursion only for positive z. We show in Fig. 2 the exact results for the functions $g_{1,2,3}(z/t, t)$ at the corresponding grid points, together with the numerical integration result for several values of $t = 0.5, 1, 2$.

How well can we expect to be able to reconstruct the functions $g_j(z, t)$ in terms of their values on a grid of uniform spacing t? We give next an estimate of the best possible interpolation error.

The simplest interpolation method of a function from its values on a uniformly spaced grid is as a cardinal series [12]. We illustrate this on the example of $g(z, t) \equiv g_0(z, t)$, which is related to the logistic-normal integral. According to this method the function $g(z, t)$ can be approximated in terms of its values at $z_k = (k + \frac{1}{2})t$ as

$$C_N(z, t) = \sum_{k=-N}^{N} g(z_k)\, \mathrm{sinc}\left(\frac{z - z_k}{t}\right) \tag{49}$$

with $\mathrm{sinc}(x) = \sin(\pi x)/(\pi x)$. By construction, the cardinal series $C_N(z, t)$ reproduces the values of $g(z, t)$ at the $2N + 1$ points $z_{-N}, \ldots, z_N$. As the number of interpolation nodes is taken to be very large, the approximation error is bounded everywhere by [13,14]

$$\lim_{N\to\infty} |g(z, t) - C_N(z, t)| \le \frac{2}{\pi} \int_{\pi/t}^{\infty} d\omega |\tilde{g}(\omega, t)|, \tag{50}$$

where $\tilde{g}(\omega, t)$ is the Fourier transform of $g(z, t)$, defined as

$$g(z, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega z} \tilde{g}(\omega, t). \tag{51}$$

In particular, if the function $g(z, t)$ is band-limited such that its Fourier transform vanishes outside the range $|\omega| \le \pi/t$, then the cardinal series converges to $g(z, t)$ itself, which is the statement of the Shannon–Whittaker sampling theorem [12]. If the function $g(z, t)$ is not band-limited, the (mis)-application of the sampling theorem introduces an aliasing error, which is bounded as shown in (50). Intuitively, this bound states that the interpolation error is small if the function $g(z, t)$ oscillates sufficiently slowly between nodes. We will use (50) as our estimate for the best attainable interpolation error from a sampling of the function $g(z, t)$ on a uniform grid of step t.

Using the explicit result for the Fourier transform of $g(z, t)$

$$\tilde{g}(\omega, t) = e^{-\frac{1}{2}\omega^2 t + \frac{1}{8}t} \frac{\pi}{\cosh \pi\omega} \tag{52}$$

we can derive an analytic upper bound on the interpolation error (50)

$$\lim_{N\to\infty} |g(z, t) - C_N(z, t)| \le \sqrt{\frac{\pi}{2t}} \frac{e^{\frac{1}{8}t}}{\cosh(\pi^2/t)} \left(1 - \mathrm{Erf}\left(\frac{\pi}{\sqrt{2t}}\right)\right). \tag{53}$$

This is an increasing function of t, which takes the value 2.5×10^{-7} at $t = 1$, 4.3×10^{-4} at $t = 2$ and 0.02 at $t = 4$. Numerical integration of (50) gives a smaller result, such that at $t = 1$ the upper bound on the error is 1.3×10^{-7}.

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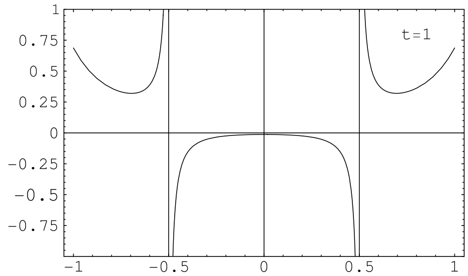

Fig. 3. The truncation error of the Poisson series. The plot shows $(g_N(z,t) - g(z,t))/g(z,t)(\times 10^4)$ at $t = 1$, where $g_N(z,t)$ is given by the Poisson summation formula with $N = 5$ terms, and $g(z,t)$ is obtained by numerical integration using trapezoidal quadrature with step $h = 0.1$.

The interpolation error is everywhere below 0.01 for $t < 3.3$ according to the analytical bound (53) and $t < 3.83$ according to the exact error bound (50). In conclusion, the function $g(z,t)$ related to the logistic-normal integral can be recovered by interpolation from its values on the grid $z_k = (k + \frac{1}{2})t$ with an error better than 1% for all $t < 3$. Similar error estimates can be obtained from (50) for all functions $g_j(z,t)$ considered above, using their Fourier transform $\tilde{g}_j(\omega,t) = (-i\partial_\omega)^j \tilde{g}(\omega,t)$ where $\tilde{g}(\omega,t)$ is given in (52).

6. Series representation by Poisson summation formula

In this section we show that an application of the Poisson summation formula [15,16] can be used to derive series expansions for the functions $\varphi^{(\pm)}(z,t)$, which can be used to obtain their values for any z. A key role in this derivation is played by the recurrence relation (31).

We illustrate the method on the simplest example of the logistic-normal integral $\varphi(z,t)$ corresponding to the case $f(x) = 1$. It is more convenient to consider the equivalent problem of deriving a series expansion for the function $g(z,t)$, defined as in (30)

$$g(z,t) = e^{\frac{1}{8}t} \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi t}} e^{-\frac{1}{2t}(x-z)^2} \frac{1}{2\cosh\frac{x}{2}}. \tag{54}$$

This is related to $\varphi(z,t)$ as

$$\varphi(z,t) = e^{-z/2} g\left(z - \frac{t}{2}, t\right). \tag{55}$$

The function $g(z,t)$ is a symmetric function in the first argument $g(-z,t) = g(z,t)$. From Eq. (54) the function $g(z,t)$ is integrable $g \in L^1$. By the results of Section 3 we know $g(z,t)$ exactly at $z_k = (k + \frac{1}{2})t$ equal to half-integer multiples of t. In particular, $g(\frac{1}{2}t, t) = g(-\frac{1}{2}t, t) = \frac{1}{2}$ is independent of t.

The function $g(z,t)$ can be represented as a Fourier integral

$$g(z,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega z} \tilde{g}(\omega,t), \tag{56}$$

with $\tilde{g}(\omega,t)$ given above in (52). Since $g(z,t)$ is integrable, we can use the Poisson summation formula to find an expression for $g(z,t)$ in terms of its Fourier transform [15,16]. The result is

$$\sum_{k=-\infty}^{\infty} g(z+kt, t) = \frac{1}{t} \sum_{j=-\infty}^{\infty} \tilde{g}\left(\frac{2\pi j}{t}, t\right) e^{\frac{2\pi i j}{t} z}. \tag{57}$$

Since the recursion relation (31) relates all the values of the function $g(z+kt,t)$ to $g(z,t)$, this relation can be used to find $g(z,t)$.

Using this approach, Eq. (57) can be put into the form

$$\begin{aligned} g(z,t) &\sum_{k=-\infty}^{\infty} (-)^k e^{-kz-\frac{1}{2}k^2 t} - \sum_{j=1}^{\infty} (-)^j \frac{\cosh[\frac{1}{2}(2j-1)z] \exp[\frac{1}{2}(j-j^2)t]}{\sinh[\frac{1}{4}(2j-1)t]} \\ &= \frac{\pi}{t} e^{t/8} \sum_{k=-\infty}^{\infty} e^{-\frac{2\pi^2}{t}k^2} \frac{\cos(\frac{2\pi z k}{t})}{\cosh(\frac{2\pi^2 k}{t})}. \end{aligned} \tag{58}$$

This expression can be used for the numerical evaluation of $g(z,t)$ and thus of the logistic-normal integral $\varphi(z,t)$.

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The series multiplying $g(z,t)$ can be written in terms of one of the Jacobi theta functions with imaginary argument as

$$\sum_{j=-\infty}^{\infty}(-)^j e^{-kz-\frac{1}{2}j^2 t} = \vartheta_4\left(\frac{i}{2}z, e^{-\frac{1}{2}t}\right), \tag{59}$$

where the function $\vartheta_4(z,q)$ is defined as [17]

$$\vartheta_4(z,q) = \sum_{n=-\infty}^{\infty}(-)^n q^{n^2}\exp(2niz). \tag{60}$$

We recall briefly a few well-known properties of the Jacobi theta function [17]: $\vartheta_4(z,q)$ is an even function in z. The argument q is usually represented as $q = e^{i\pi\tau}$ where the imaginary part of τ is chosen to be positive. The function $\vartheta_4(z,q)$ has zeros at $z_0 = \frac{1}{2}\pi\tau + m\pi + n\pi\tau$, with $(m,n) \in \mathbb{Z}$.

For our case $\tau = \frac{it}{2\pi}$, such that the series (59) vanishes at the points

$$z_{m,n} = \frac{1}{2}t + m2\pi i + nt, \qquad (m,n) \in \mathbb{Z}. \tag{61}$$

These points form the nodes of a lattice with periods $(t, 2\pi i)$. In particular, (59) vanishes at the points $z = \pm\frac{1}{2}t$, such that at these points the expression (58) has 0/0 form, but with a finite and known limit given in (20).

What is the numerical precision of the evaluation of the logistic-normal integral $g(z,t)$ from the Poisson series formula (58)? Denote $\bar{g}_N(z,t)$ the approximation obtained by truncating the sums over (k,j) in (58) as $k = (-N,N)$ and $j = (1,N)$. This will be compared to the numerical evaluation of $g(z,t)$ by trapezoidal quadrature with step $h = 0.1$. According to Eq. (6) the approximation error $|E(h)|$ is a decreasing function of time, which is bounded at $t = 1$ as $|E(h)| \le 10^{-42}$. We will use this as the benchmark numerical evaluation against which the performance of the Poisson series (58) will be measured.

We study the relative truncation error $\Delta g_N(z,t) = (\bar{g}_N(z,t) - g(z,t))/g(z,t)$ as function of z at fixed time t. In Fig. 3 we show the truncation error for the Poisson summation formula with $t = 1$ keeping $N = 5$ terms in the sum. The error is very small in the middle of the interval at $z = 0$, and increases towards the edges of the interval $z = \pm t/2$. This is due to the fact that, as mentioned, the coefficient of $g(z,t)$ in (58) vanishes at these points, which leads to numerical instability. Fortunately, at these points the values of $g(z,t)$ are exactly known from the recursion relation, and can be obtained from (20).

The numerical performance of the Poisson series (58) is optimal at $z = 0$. The truncation error at $z = 0$ and $t = 1$ is $\Delta g_N(0,1) \sim -1.3 \times 10^{-6}$ with $N = 5$, and decreases to less than 10^{-14} by keeping $N = 10$ terms in the sum. Thus the Poisson series expansion based on Eq. (58) gives an efficient method for evaluating the logistic-normal integral $g(z,t)$ at arbitrary points within the $z = (-t/2, t/2)$ interval. These values can be combined with the exactly known values at $z = \pm\frac{1}{2}t$ to obtain a precise determination of this function.

7. Concluding comments

The method of the recurrence relations for the solutions of the one-dimensional heat equation considered in this note can be used to find exact results for cases which are not tractable analytically by other methods. We have shown that it can be used to find exact results for the solution of the heat equation with initial condition of the form $f(x)/(1+\exp(\sigma x))$ on a grid of equidistant points of width σt. These values can be used in practice for a numerical evaluation of the full solution by interpolation from the grid values, using for example spline interpolation, or the cardinal series as shown in Section 5.

The practical utility of the method proposed here depends on the relative size of the grid width σt, and the spatial variation of the function $f(x)$ between the grid points. The logistic-normal integral $\varphi(z,t)$, for which $f(x) = 1$ is a constant, can be approximated from its exactly known values on the grid $z_k = kt$ with an error below 1% for all $t < 3.8$, as shown in Section 5. For larger t, one can construct a precise approximation of $\varphi(z,t)$ within the quasi-period $(0,t)$ using the exactly known values on the boundaries, and at a few interior points using the Poisson summation method of Section 6. The resulting approximation can be extended to any other point by repeated application of the recurrence relation (16).

We would like to find an estimate for the error of such an approximation. Consider the approximation $\bar{\varphi}(z,t)$ of the logistic-normal integral $\varphi(z,t)$ with the following properties: it reproduces the exactly known values at $z = 0, t$

$$\bar{\varphi}(0,t) = \frac{1}{2}, \qquad \bar{\varphi}(t,t) = \frac{1}{2}e^{-\frac{1}{2}t} \tag{62}$$

and outside the interval $(0,t)$ the approximation $\bar{\varphi}(z,t)$ is defined by repeated application of Eq. (16).

Using the recurrence relation (16) we find that the approximation error $\Delta\varphi(z,t) \equiv \varphi(z,t) - \bar{\varphi}(z,t)$ satisfies the recurrence relation

$$\Delta\varphi(z+t,t) = -e^{-z-\frac{1}{2}t}\Delta\varphi(z,t). \tag{63}$$

The most general solution of this relation has the form

$$\Delta\varphi(z,t) = h(z,t)e^{-\frac{1}{2t}z^2}, \tag{64}$$

where $h(z,t)$ is antiperiodic in the first argument with period t

$$h(z+t,t) = -h(z,t). \tag{65}$$

This implies that the approximation error is largest in the vicinity of $z = 0$, and decreases rapidly away from this point. The approximation error is bounded everywhere by

$$|\Delta\varphi(z,t)| \leq e^{-\frac{1}{2t}z^2+\frac{1}{8}t} \sup(|\Delta\varphi(z,t)|; z \in (0,t)). \tag{66}$$

Although we considered here for definiteness the logistic-normal integral, the argument applies equally well for any arbitrary $\varphi(z,\sigma,t)$ as given by (4) for which $f(z,t)$ can be evaluated in closed form.

Generally the method proposed in this paper can be used if the function $f(z,t)$ is sufficiently slow varying on the scale of the grid spacing. Of course, if additional points are needed, one can always refine the grid by computing numerically the value of $\varphi(z,\sigma,t)$ at one intermediate point z_0, and using the recurrence relations to obtain the value of the function on the grid $z_0 + k\sigma t$ with $k \in \mathbb{Z}$.

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References

[1] L.C. Evans, Partial Differential Equations, in: Graduate Studies in Mathematics, vol. 19, American Mathematical Society, 2002.
[2] J.F. Monahan, L.A. Stefanski, in: N. Balakrishnan (Ed.), Handbook of the Logistic Distribution, Marcel Dekker, New York, 1992.
[3] E. Demidenko, Mixed Models: Theory and Applications, Wiley-Interscience, Hoboken, 2004.
[4] P. Maragakis, et al., Bayesian estimates of free energies from nonequilibrium work data in the presence of instrument noise, J. Chem. Phys. 129 (2008) 024102.
[5] E. Crouch, D. Spiegelman, The evaluation of integrals of the form $\int_{-\infty}^{\infty} dtf(t)\exp(-t^2)$: application to logistic-normal models, J. Amer. Statist. Assoc. 85 (1990) 464–469.
[6] E.T. Goodwin, The evaluation of integrals of the form $\int_{-\infty}^{\infty} dxf(x)\exp(-x^2)$, Proc. Cambridge Philos. Soc. 45 (1949) 241–245.
[7] F. Black, E. Derman, W. Toy, A one-factor model of interest rates and its application to treasury bond options, Financ. Anal. J. (1990) 24–32.
[8] F. Black, P. Karasinski, Bond and option pricing when short rates are lognormal, Financ. Anal. J. (1991) 52–59.
[9] F. Jamshidian, Forward induction and construction of yield curve diffusion models, J. Fixed Income 1 (1991) 62–74.
[10] P.J. Schönbucher, Credit Derivatives Pricing Models: Model, Pricing and Implementation, Wiley, 2003.
[11] D.V. Widder, The Heat Equation, Academic Press, 1975.
[12] J.P. Boyd, Chebyshev and Fourier Spectral Methods, Dover Publishers, 2001.
[13] P. Weiss, An estimate for the error arising from the misapplication of the sampling formula, Notices Amer. Math. Soc. 10 (1963) 35.
[14] J.L. Brown, On the error in reconstructing a non-bandlimited function by means of the bandpass sampling theorem, J. Math. Anal. Appl. 18 (1967) 75–84.
[15] R. Courant, D. Hilbert, Methods of Mathematical Physics, V.1, Interscience Publishers, New York, 1953.
[16] S. Sternberg, Theory of functions of a real variable, 2005.
[17] E.T. Whittaker, G.N. Watson, A Course of Modern Analysis, Cambridge University Press, 1927.

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