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ANALYSIS OF THE RANDOM HEAT EQUATION *VIA* APPROXIMATE DENSITY FUNCTIONS

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Abstract. In this paper we study the randomized heat equation with homogeneous boundary conditions. The diffusion coefficient is assumed to be a random variable and the initial condition is treated as a stochastic process. The solution of this randomized partial differential equation problem is a stochastic process, which is given by a random series obtained *via* the classical method of separation of variables. Any stochastic process is determined by its finite-dimensional joint distributions. In this paper, the goal is to obtain approximations to the probability density function of the solution (the first finite-dimensional distributions) under mild conditions. Since the solution is expressed as a random series, we perform approximations to its probability density function. Several illustrative examples are shown.

Key words: Random heat equation, Random Variable Transformation technique, Probability density function.

1. INTRODUCTION

Differential equations governing real phenomena contain some mathematical terms (*e.g.*, initial/boundary condition, source term, coefficients), referred to as model parameters, that characterize physical features of the problem and its environment. In practice, these terms must be determined from sampling and/or experimentally. Hence they contain errors coming from different sources such as the lack of accuracy in sampling and/or measurements and the inherent uncertainty usually met in complex physical phenomena. In that case, it is more convenient to treat constants and functions playing the role of model parameters as random variables and stochastic processes, respectively. This approach leads to Random Differential Equations (RDEs). RDEs consist in a direct randomization of all model parameters subject to uncertainty through random variables and/or stochastic processes having regular trajectories. This approach allows for a wide range of random patterns (binomial, Poisson, hypergeometric, beta, exponential, Gaussian, etc.) [1].

In dealing with RDEs defined in a complete probability space, say $(\Omega, \mathcal{F}, \mathbb{P})$, as it also happens in the deterministic scenario, the primary objective is to compute exact or numerically their solution, say $u(x) = u(x)(\omega)$, $\omega \in \Omega$, which is a stochastic process instead of a classical function. A distinctive feature of solving RDEs, with respect to their deterministic counterpart, is the need to compute relevant probabilistic information of the solution, such as the mean function, $\mathbb{E}[u(x)]$, and the variance function, $\mathbb{V}[u(x)]$. While a more and complex ambitious goal is to determine the finite-dimensional probability distributions, particularly the so-called first probability density function, say $f(u,x)$, associated to the solution, since from it one can compute any one-dimensional statistical moment. Furthermore, the computation of $f(u,x)$ permits calculating the probability that the solution stochastic process lies within an interval of interest, say $[u_1,u_2]$.

The heat equation is a differential statement of thermal energy balance law. It is a basic model to numerous physical phenomena such as diffusion, heat conduction, transport of solutes, etc., but it has also been successfully applied in other apparently unrelated areas like finance to pricing security derivatives traded in the stock market [2, 3]. Impurities and heterogeneity in the medium (cross section) and error measurements justify the consideration of randomness in both the diffusion coefficient and the initial condition. This motivates us to study the randomized heat equation defined on a finite spatial domain whose diffusion coefficient is assumed to be a random variable, the boundary conditions are homogeneous and the initial condition is a stochastic process. Different randomizations of the heat equation have been studied in the existing literature using different techniques, such as generalized polynomial chaos based stochastic Galerkin technique [4], homogenization and Monte Carlo approaches [5], random mean square calculus [6], random collocation method [7], random interval moment method [8], Kolmogorov's criterion [9], etc.

Our approach is based upon RDEs and our main goal is to construct reliable approximations to the probability density function of the solution (the first finite-dimensional distributions) under mild conditions. To achieve this target we will employ the Random Variable Transformation (RVT) technique. In the context of RDEs, the RVT technique has been successfully applied to compute the probability density function of the solution to significant problems in Physics, Biology, etc., assuming specific distributions for the model parameters [10–13] or dealing with general parametric distributions [14].

The heat problem that we are going to deal with is the following:

$$\begin{cases} u_t = \alpha^2 u_{xx}, \quad 0 < x < 1,\, t > 0, \\ u(0,t) = u(1,t) = 0, \quad t \geq 0, \\ u(x,0) = \phi(x), \quad 0 \leq x \leq 1. \end{cases} \tag{1}$$

We consider (1) in a random setting, meaning that we are going to work on an underlying complete probability space $(\Omega,\mathcal{F},\mathbb{P})$, where Ω is the set of outcomes, that will be generically denoted by ω, $\mathcal{F}$ is a σ-algebra of events and $\mathbb{P}$ is a probability measure. We consider the diffusion coefficient $\alpha^2(\omega)$ as a positive random variable and the initial condition $\phi = \{\phi(x)(\omega) : 0 \le x \le 1, \omega \in \Omega\}$ as a stochastic process in our probability space. The solution to (1) is a stochastic process expressed as a formal random series,

$$u(x,t)(\omega) = \sum_{n=1}^{\infty} A_n(\omega)\, \mathrm{e}^{-n^2\pi^2\alpha^2(\omega)t} \sin(n\pi x), \tag{2}$$

where the random Fourier coefficient

$$A_n(\omega) = 2\int_0^1 \phi(y)(\omega) \sin(n\pi y)\, \mathrm{d}y \tag{3}$$

is understood as a Lebesgue integral, for each $\omega \in \Omega$ fixed (sample path integral).

Notice that if $\phi(\cdot)(\omega) \in \mathrm{L}^1(0,1)$, then

$$|A_n(\omega)\, \mathrm{e}^{-n^2\pi^2\alpha^2(\omega)t} \sin(n\pi x)| \le 2\|\phi(\cdot)(\omega)\|_{\mathrm{L}^1(0,1)} \mathrm{e}^{-n^2\pi^2\alpha^2(\omega)t},$$

so by the comparison and the D'Alembert tests the random series given in (2) is almost surely convergent and $u(x,t)(\omega)$ is well-defined, for $0 < x < 1$ and $t > 0$.

The main goal of this paper is, under suitable hypotheses, to compute approximations of the probability density function of the solution $u(x,t)(\omega)$ given in (2), for $0 < x < 1$ and $t > 0$.

We end the introduction by recalling the RVT technique. The RVT technique gives the density function of a response Y under the relation output-input $Y = g(X)$, where g is a deterministic map, called the transformation mapping, and X is a random quantity. It is assumed that the dimensions of X and Y are equal.

Lemma 1 *(Random Variable Transformation (RVT) technique) [15, p. 47] Let X be an absolutely continuous random vector with density f_X and with support D_X contained in an open set $D \subseteq \mathbb{R}^n$. Let $g : D \to \mathbb{R}^n$ be a $C^1(D)$ function, injective on D such that $Jg(x) \neq 0$ for all $x \in D$ (J stands for Jacobian). Let $h = g^{-1} : g(D) \subset \mathbb{R}^n \to \mathbb{R}^n$. Let $Y = g(X)$ be a random vector. Then Y is absolutely continuous with density*

$$f_Y(y) = \begin{cases} f_X(h(y))|Jh(y)|, & y \in g(D), \\ 0, & y \notin g(D). \end{cases} \tag{4}$$

2. COMPUTATION OF THE PROBABILITY DENSITY FUNCTION

The following result provides general sufficient conditions so that the probability density function of $u(x,t)$ can be approximated. Since $u(x,t)$ depends on infinitely many random variables, α^2, $A_1, A_2, \ldots$, we truncate the infinite series to a finite order N, so that we achieve a transformation of α^2, $A_1, \ldots, A_N$. The RVT method allows for computing the density function of such transformation. When $N \to \infty$, we expect convergence to the true density function of $u(x,t)$.

Theorem 2 *Suppose that α^2, A_1 and $(A_2,\ldots,A_N)$ are independent and absolutely continuous random variables, for $N \geq 2$. Suppose that the probability density function f_{A_1} is almost everywhere continuous on $\mathbb{R}$, bounded on $\mathbb{R}$, and $\mathbb{E}[\mathrm{e}^{\pi^2\alpha^2 t}] < \infty$. Then the density of $u_N(x,t)(\omega) = \sum_{n=1}^N A_n(\omega)\,\mathrm{e}^{-n^2\pi^2\alpha^2(\omega)t}\sin(n\pi x)$,*

$$f_{u_N(x,t)}(u) = \int_{\mathbb{R}^N} f_{A_1}\left(\frac{\mathrm{e}^{\pi^2\alpha^2 t}}{\sin(\pi x)}\left\{u - \sum_{n=2}^N a_n \mathrm{e}^{-n^2\pi^2\alpha^2 t}\sin(n\pi x)\right\}\right)$$
$$\times f_{(A_2,\ldots,A_N)}(a_2,\ldots,a_N) f_{\alpha^2}(\alpha^2)\frac{\mathrm{e}^{\pi^2\alpha^2 t}}{\sin(\pi x)}\,\mathrm{d}a_2\cdots\mathrm{d}a_N\,\mathrm{d}\alpha^2, \tag{5}$$

converges pointwise to the density of the random variable $u(x,t)(\omega)$ given by (2), for $0 < x < 1$ and $t > 0$. There is also convergence in $\mathrm{L}^1(\mathbb{R};\mathrm{d}u)$.

Proof. Let

$$g(A_1,\ldots,A_N,\alpha^2) = \left(\sum_{n=1}^N A_n \mathrm{e}^{-n^2\pi^2\alpha^2 t}\sin(n\pi x), A_2,\ldots,A_N,\alpha^2\right).$$

In the notation of Lemma 1, $D = \mathbb{R}^{N+1}$, $g(D) = \mathbb{R}^{N+1}$,

$$h(A_1,\ldots,A_N,\alpha^2) = \left(\frac{\mathrm{e}^{\pi^2\alpha^2 t}}{\sin(\pi x)}\left\{A_1 - \sum_{n=2}^N A_n \mathrm{e}^{-n^2\pi^2\alpha^2 t}\sin(n\pi x)\right\}, A_2,\ldots,A_N,\alpha^2\right)$$

and

$$Jh(A_1,\ldots,A_N,\alpha^2) = \frac{\mathrm{e}^{\pi^2\alpha^2 t}}{\sin(\pi x)} > 0.$$

Then, as a consequence of the RVT formula (4),

$$f_{(u_N(x,t),A_2,\ldots,A_N,\alpha^2)}(u,a_2,\ldots,a_N,\alpha^2)$$
$$= f_{(A_1,\ldots,A_N,\alpha^2)}\left(\frac{\mathrm{e}^{\pi^2\alpha^2 t}}{\sin(\pi x)}\left\{u - \sum_{n=2}^N a_n \mathrm{e}^{-n^2\pi^2\alpha^2 t}\sin(n\pi x)\right\}, a_2,\ldots,a_N,\alpha^2\right)\frac{\mathrm{e}^{\pi^2\alpha^2 t}}{\sin(\pi x)}.$$

Computing marginals, we derive (5):

$$f_{u_N(x,t)}(u) = \int_{\mathbb{R}^N} f_{(u_N(x,t),A_2,\ldots,A_N,\alpha^2)}(u,a_2,\ldots,a_N,\alpha^2)\,\mathrm{d}a_2\cdots\mathrm{d}a_N\,\mathrm{d}\alpha^2.$$

From (5) and the independence between α^2, A_1 and $(A_2,\ldots,A_N)$, notice that

$$f_{u_N(x,t)}(u) = \frac{1}{\sin(\pi x)}\mathbb{E}\left[f_{A_1}\left(\frac{\mathrm{e}^{\pi^2\alpha^2 t}}{\sin(\pi x)}\left\{u - \sum_{n=2}^N a_n \mathrm{e}^{-n^2\pi^2\alpha^2 t}\sin(n\pi x)\right\}\right)\mathrm{e}^{\pi^2\alpha^2 t}\right].$$

Since f_{A_1} is almost everywhere continuous on $\mathbb{R}$, the continuous mapping theorem

[16, p. 7, Th. 2.3] implies

$$\lim_{N\to\infty} f_{A_1}\left(\frac{e^{\pi^2\alpha^2 t}}{\sin(\pi x)}\left\{u-\sum_{n=2}^{N} a_n e^{-n^2\pi^2\alpha^2 t}\sin(n\pi x)\right\}\right)$$
$$= f_{A_1}\left(\frac{e^{\pi^2\alpha^2 t}}{\sin(\pi x)}\left\{u-\sum_{n=2}^{\infty} a_n e^{-n^2\pi^2\alpha^2 t}\sin(n\pi x)\right\}\right)$$

almost surely. On the other hand,

$$\left| f_{A_1}\left(\frac{e^{\pi^2\alpha^2 t}}{\sin(\pi x)}\left\{u-\sum_{n=2}^{N} a_n e^{-n^2\pi^2\alpha^2 t}\sin(n\pi x)\right\}\right)\right| e^{\pi^2\alpha^2 t}$$
$$\le \|f_{A_1}\|_\infty e^{\pi^2\alpha^2 t} \in \mathrm{L}^1(\Omega; \mathrm{d}\mathbb{P}).$$

By the dominated convergence theorem [17, result 11.32, p. 321], we can interchange the limit with respect to N and the expectation:

$$\lim_{N\to\infty} f_{u_N(x,t)}(u) = \frac{1}{\sin(\pi x)}\mathbb{E}\left[f_{A_1}\left(\frac{e^{\pi^2\alpha^2 t}}{\sin(\pi x)}\left\{u-\sum_{n=2}^{\infty} a_n e^{-n^2\pi^2\alpha^2 t}\sin(n\pi x)\right\}\right) e^{\pi^2\alpha^2 t}\right]$$
$$= f_{u(x,t)}(u).$$

This proves the pointwise convergence.

Finally, convergence in $\mathrm{L}^1(\mathbb{R}; \mathrm{d}u)$ follows from Scheffé's Lemma [18, p. 55], [19].

□

In the following examples, we detail some cases where the hypotheses of Theorem 2 hold.

Example 1 If $\phi(x) = B(x)$, where B is a standard Brownian bridge on $[0,1]$ [20], then $A_1, A_2, \ldots$ are independent, and we are in position of applying Theorem 2. Indeed, by [20, Lemma 5.22] we know that $\mathbb{C}\mathrm{ov}[B(y), B(z)] = \min\{y,z\} - yz$, hence

$$\mathbb{C}\mathrm{ov}[A_n, A_m] = 4\int_0^1\int_0^1 (\min\{y,z\} - yz)\sin(n\pi y)\sin(m\pi z)\,\mathrm{d}y\,\mathrm{d}z$$
$$= \begin{cases} 0, & n \neq m, \\ \frac{2}{n^2\pi^2}, & n = m, \end{cases}$$

for $1 \le n, m \le N$, and since $(A_1, \ldots, A_N)$ is multivariate Gaussian for all $N \ge 1$, then by [20, Lemma 4.33] independence of $A_1, A_2, \ldots$ follows. Notice that we have used that A_n, $1 \le n \le N$, defined by (3), are Gaussian, [1, Th. 4.6.4], since $B(x)$ is Gaussian for each $0 \le x \le 1$, [20, p. 193].

Recall that the Brownian bridge has zero values at $x = 0$ and $x = 1$, so it does make sense to model the initial condition *via* such process.

Continuing with the computations, we have $A_1, A_2, \ldots$ independent and $A_n \sim \text{Normal}(0, 2/(n^2\pi^2))$ for $n \geq 1$, so

$$f_{(A_1,\ldots,A_N)}(a_1,\ldots,a_N) = \left(\frac{\sqrt{\pi}}{2}\right)^N \prod_{n=1}^{N} n\,\mathrm{e}^{-\frac{n^2\pi^2 a_n^2}{4}}.$$

Thus,

$$f_{u_N(x,t)}(u) = \left(\frac{\sqrt{\pi}}{2}\right)^N \int_{\mathbb{R}^N} \mathrm{e}^{-\frac{\pi^2}{4}\frac{\mathrm{e}^{2\pi^2\alpha^2 t}}{\sin^2(\pi x)}\left\{u - \sum_{n=2}^{N} a_n \mathrm{e}^{-n^2\pi^2\alpha^2 t}\sin(n\pi x)\right\}^2} \times \left(\prod_{n=2}^{N} n\,\mathrm{e}^{-\frac{n^2\pi^2 a_n^2}{4}}\right) f_{\alpha^2}(\alpha^2)\frac{\mathrm{e}^{\pi^2\alpha^2 t}}{\sin(\pi x)}\,\mathrm{d}a_2\cdots\mathrm{d}a_N\,\mathrm{d}\alpha^2. \tag{6}$$

Example 2 Let ϕ be a process of the following form:

$$\phi(x)(\omega) = \sum_{j=1}^{\infty} \sqrt{\nu_j}\,\sqrt{2}\sin(j\pi x)\,\xi_j(\omega), \tag{7}$$

where the sum is considered in the topology of $\mathrm{L}^2([0,1]\times\Omega)$, $\{\nu_j\}_{j=1}^{\infty}$ are positive real numbers satisfying $\sum_{j=1}^{\infty}\nu_j < \infty$, and $\{\xi_j\}_{j=1}^{\infty}$ are absolutely continuous random variables with zero expectation, unit variance and independent. Notice that the sum is well-defined in $\mathrm{L}^2([0,1]\times\Omega)$, because for two indexes $N > M$ we have, by Pythagoras theorem in $\mathrm{L}^2([0,1]\times\Omega)$,

$$\begin{aligned}\left\|\sum_{j=M+1}^{N}\sqrt{\nu_j}\,\sqrt{2}\sin(j\pi x)\,\xi_j\right\|^2_{\mathrm{L}^2([0,1]\times\Omega)} &= \sum_{j=M+1}^{N}\nu_j\,\|\sqrt{2}\sin(j\pi x)\|^2_{\mathrm{L}^2([0,1])}\|\xi_j\|^2_{\mathrm{L}^2(\Omega)}\\ &= \sum_{j=M+1}^{N}\nu_j \overset{N,M\to\infty}{\longrightarrow} 0,\end{aligned}$$

since $\|\xi_j\|^2_{\mathrm{L}^2(\Omega)} = \mathbb{V}[\xi_j] = 1$ and

$$\|\sqrt{2}\sin(j\pi x)\|^2_{\mathrm{L}^2([0,1])} = 2\int_0^1 \sin^2(j\pi x)\,dx = 1 - \frac{\sin(2\pi j)}{2\pi j} = 1, \quad j = 1, 2, \ldots.$$

Expression (7) for ϕ is very intuitive: as we require $\phi(0) = \phi(1) = 0$, the orthonormal basis to work with in order to expand $\phi(\cdot)(\omega)$ as a random Fourier series is $\{\sqrt{2}\sin(j\pi x)\}_{j=1}^{\infty}$. In this way,

$$\phi(x)(\omega) = \sum_{j=1}^{\infty} c_j(\omega)\,\sqrt{2}\sin(j\pi x).$$

Expression (7) corresponds to the Karhunen-Loève expansion [20]. Some recent contributions where the Karhunen-Loève expansion is applied to solve relevant problems in Physics can be found in [21, 22].

If ϕ has expression (7) and the density function f_{ξ_1} is almost everywhere continuous and bounded on $\mathbb{R}$, then the hypotheses of Theorem 2 hold. Indeed,

$$\begin{aligned} A_n(\omega) &= 2\int_0^1 \phi(y)(\omega)\sin(n\pi y)\,dy = 2\sum_{j=1}^{\infty}\sqrt{\nu_j}\,\sqrt{2}\int_0^1 \sin(j\pi y)\sin(n\pi y)\,dy\,\xi_j(\omega) \\ &= \sqrt{2}\,\sqrt{\nu_n}\,\xi_n(\omega), \end{aligned} \tag{8}$$

so $A_1, A_2, \ldots$ are absolutely continuous and independent random variables, which gives the condition of Theorem 2. Thus, one may use formula (5), $f_{u_N(x,t)}(u)$, to approximate the density of the solution $u(x,t)(\omega)$ given in (2), whenever ϕ has the form (7) and the rest of hypotheses in Theorem 2 hold.

3. NUMERICAL EXAMPLES

In this section we put specific probability distributions for α^2 and ϕ, and we approximate the probability density function of $u(x,t)$ at different space-time locations. We use orders of truncation N for the approximations.

Example 3 Consider the randomized PDE problem (1), with $\alpha^2 \sim \text{Uniform}(1,2)$ and $\phi(x) = B(x)$ a standard Brownian bridge on $[0,1]$, being both independent random variables for each $x \in [0,1]$. The hypotheses of Theorem 2 are satisfied. We will perform numerical approximations to the probability density function of the solution $u(x,t)(\omega)$ given by (2). For that purpose, we will use formula (6), which gives $f_{u_N(x,t)}(u)$.

In Figure 1, we show the density $f_{u_N(x,t)}(u)$ given by (5) for $N = 2$ and $N = 3$, $x = 0.5$ and at different time instants $t = 0.05, 0.1, 0.15, 0.3$. For these orders N, we have a double and a triple integral, respectively, computable by means of quadrature rules. Observe that similar densities are plotted for $N = 2$ and $N = 3$, showing rapid convergence with N.

Notice that, as t increases, the density of $u(x,t)(\omega)$ seems to behave as a Dirac delta function. Indeed, as $A_1, A_2, \ldots$ are independent and $A_n \sim \text{Normal}(0, 2/(n^2\pi^2))$, then

$$\mathbb{E}[u(x,t)] = \sum_{n=1}^{\infty}\mathbb{E}[A_n]\mathbb{E}[\mathrm{e}^{-n^2\pi^2\alpha^2 t}]\sin(n\pi x) = 0$$

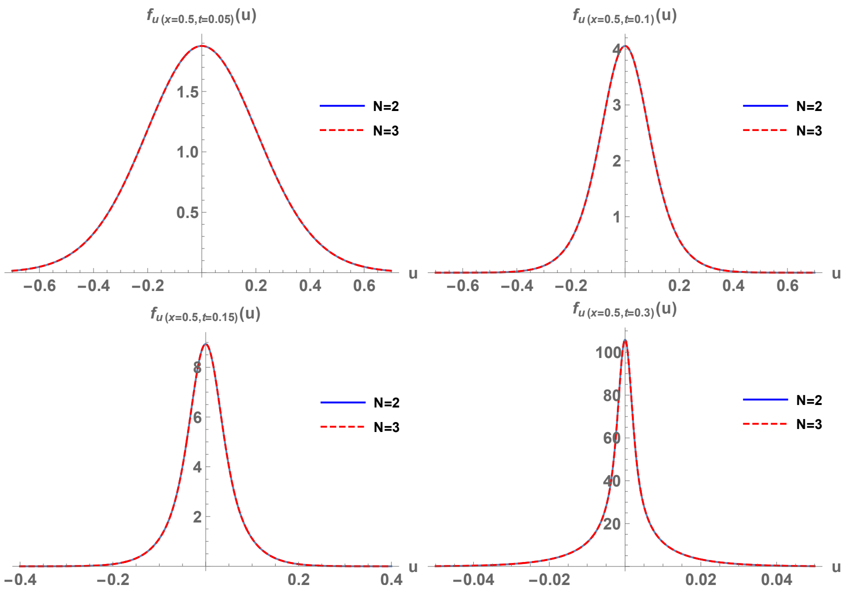

Fig. 1 – Approximations to $f_{u(x,t)}(u)$ for different orders of truncation and space-time positions, Example 3.

since $\mathbb{E}[A_n]=0$ for all $n=1,2,\ldots$ and, taking into account that $\alpha^2(\omega)\geq 1$,

$$\mathbb{V}[u(x,t)] \leq \left\| \sum_{n=1}^{\infty} |A_n|\,\mathrm{e}^{-n^2\pi^2 t} \right\|^2_{\mathrm{L}^2(\Omega)} = \sum_{n=1}^{\infty} \|A_n\|^2_{\mathrm{L}^2(\Omega)}\,\mathrm{e}^{-2n^2\pi^2 t}$$
$$= \sum_{n=1}^{\infty} \frac{2}{n^2\pi^2}\mathrm{e}^{-2n^2\pi^2 t} \stackrel{t\to\infty}{\longrightarrow} 0.$$

Therefore, the density tends to be concentrated around zero.

Example 4 Let

$$\phi(x)(\omega) = \sum_{j=1}^{\infty} \frac{\sqrt{2}}{j^{\frac{3}{2}}\sqrt{1+\log j}} \sin(j\pi x)\xi_j(\omega)$$

be a specific Karhunen-Loève expansion (see Example 2), where $\nu_j = 1/(j^3(1+\log j))$, and $\xi_1,\xi_2,\ldots$ are identically distributed and independent, with $f_{\xi_1}(\xi_1) = \sqrt{2}/(\pi(1+\xi_1^4))$ (it can be checked that f_{ξ_1} is a density function, such that its expectation is 0 and its variance is 1). Let $\alpha^2 \sim \mathrm{Uniform}(1,2)$. Figure 2 draws the density functions for orders $N=2$ and $N=3$ and different space-time positions. Similar results are perceived with respect to N.

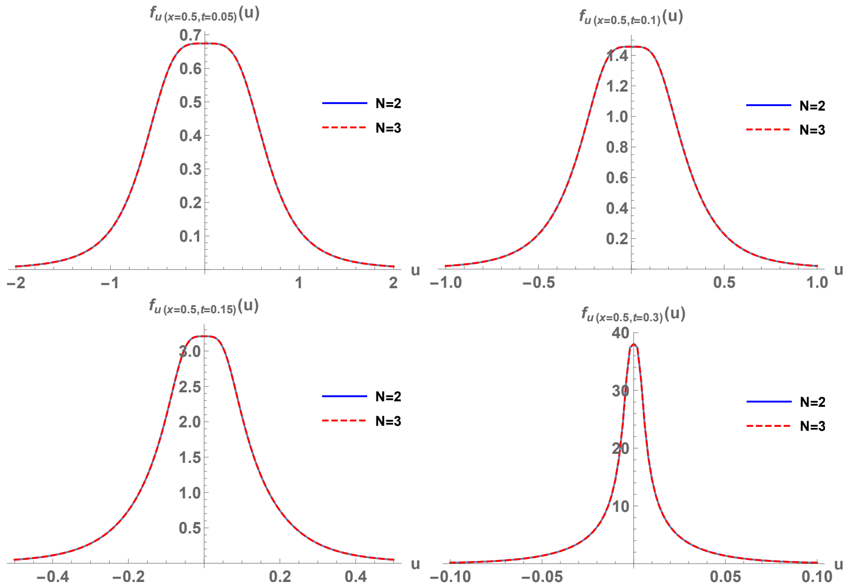

Fig. 2 – Approximations to $f_{u(0.5,t)}(u)$ for different orders of truncation at different time instants $t = 0.05, 0.1, 0.15, 0.3$. Example 4.

4. CONCLUSIONS

In this paper we have determined approximations to the probability density function of the solution to the randomized heat equation with homogeneous boundary conditions. This solution is a stochastic process expressed as a random series, which is obtained *via* the classical method of separation of variables. The random series has been truncated, and the probability density function of the finite-term sum has been computed *via* the RVT technique. A theorem guarantees the convergence of these density functions to the target density when the truncation tends to infinity. Some numerical examples with specific probability distributions have illustrated the approximations to the target density function.

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