Global Journal of Pure and Applied Mathematics.
ISSN 0973-1768 Volume 11, Number 6 (2015), pp. 4325-4337

http://www.ripublication.com/gjpam.htm

Stable reconstruction of initial condition for fractional diffusion equations[1]

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Abstract

We present a numerical method based on Tikhonov regularization for the backward problem of determining the initial condition of a fractional heat equation from noisy interior measurements. Such problem arises in a diverse set of areas with applications in environmental engineering, hydrology, and physics. To overcome the instability issue of the problem, we utilize a Tikhonov regularization scheme using the eigenfunction expansion of the forward solution, and the Generalized cross-validation method as parameter selection strategy. Numerical examples are included to validate the effectiveness of the method.

AMS subject classification: 65F22, 47A52, 35R11, 35R30, 35R25, 47J06.
Keywords: Inverse problems, Regularization, Stability, Initial distribution, Fractional diffusion, Anomalous diffusion, Generalized cross-validation.

1. Introduction

In this paper we are concerned with the inverse problem of reconstructing the initial condition for the fractional heat equation

$$\frac{\partial^\alpha u}{\partial t^\alpha}(x,t) = \frac{1}{w(x)}\frac{\partial}{\partial x}\left(q(x)\frac{\partial u}{\partial x}(x,t)\right) + f(x,t), \quad (x,t) \in \Lambda_x \times \Lambda_t, \tag{1.1}$$

supplied with the initial and boundary conditions:

$$\begin{aligned} u(x,0) &= p(x), \;\; x \in \Lambda_x, \\ u(a,t) &= u(b,t) = 0, \;\; t \in \overline{\Lambda_t}, \end{aligned} \tag{1.2}$$

[1]It was supported by the Scientific Research and Graduate Studies at Yarmouk University.

where $\Lambda_x = (a, b)$ and $\Lambda_t = (0, T]$. We assume the order of the fractional derivative is $\alpha \in (0, 1)$, and the time-fractional derivative is taken in the Caputo sense. Such equations are prototypes of what is known throughout the literature as *fractional diffusion equations*.

The problem of finding the temperature u from given source f, thermal conductivity q, and initial temperature distribution p is usually termed as *forward* or *direct problem*. In this work, we are concerned with the *inverse problem*.

Inverse Problem: Estimate $p|_{\Lambda_x}$ from noisy interior measurement u^m of $u(\overline{x}, t)$.

Here we assume that f and q are known exactly, $t \in \overline{\Lambda_t}$, and $\overline{x} \in \Lambda_x$ is a fixed location at which the data u^m is observed. Such inverse problem arises in many applications, such as, image deblurring, reconstructing the initial temperature or concentration of a contaminant in a sub-diffusive media which is relevant in environmental engineering, hydrology, and physics.

There are several but nonequivalent definitions of fractional derivatives. We adopt the Caputo definition which, in our context, is given by [1]:

$$\frac{\partial^\alpha u}{\partial t^\alpha}(\cdot, t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} \frac{\partial u(\cdot, s)}{\partial s}\, ds, \quad 0 < \alpha < 1,$$

When $\alpha = 1$, equation (1.1) reduces to the classical heat (diffusion) equation, where as, it becomes the classical Helmholtz equation for the case $\alpha = 0$. More about the theory and applications of fractional derivatives calculus can be found in [1, 2, 3].

Fractional diffusion equations are derived by considering continuous time random walk problems, which are in general non-Markovian processes. The physical interpretation of the fractional derivative is that it represents a degree of memory in the diffusing material. Therefore, such equations are very adequate in modeling slow propagation phenomena (sub-diffusion) which have been observed for example in transport processes in porous media, protein diffusion within cells, movement of a material along fractals, etc., see [3, 4, 5, 6, 7]. For the analytical and numerical aspects of the forward problem and its variations, we refer the reader to the articles [1, 2, 8, 9].

There are considerable publications treating inverse problems related to (1.1)–(1.2). In [10], Murio used regularization by mollification technique to stabilize the inverse problem of determining the temperature $u(1, t)$ and the heat flux $u_x(1, t)$ from the data $u(0, t)$ and $u_x(0, t)$. The mollified problem is then numerically solved using an adaptive space marching finite difference scheme. Zhang and Xu [11] considered the problem of identifying the time-independent source term f from the boundary data $u(0, \cdot)$. They established uniqueness results and deduced analytical solution based on the method of eigenfunction expansion. In [12], Wang and Liu considered the inverse problem of the determination of the initial distribution from internal measurements of $u(\cdot, T)$, they used total variation regularization to obtain stable approximations of the backward problem. They presented some example related to image de-blurring. Deng and Yang [13] proposed a numerical method based on the idea of reproducing kernel approximation to reconstruct the unknown initial heat distribution from a finite set of scattered measurements of transient temperature at a fixed final time. In [14], Ye and Xu formulated the inverse problem as an optimal control problem to obtain a space-time spectral method. They derived optimality conditions and some error bounds based on the weak formulation of the forward problem. See also [15, 16, 17] for other related inverse problems and their numerical and analytical treatments.

To handle the instability issue of the aforementioned inverse problem we use a Tikhonov regularization scheme in conjunction with the eigenfunction expansion of the forward solution which is derived in Section 2; the precise formulation will be given in Section 3. We present numerical examples to show the efficiency of the proposed approach.

The rest of the paper is organized as follows. In Section 2 we introduce some definitions and preliminary results concerning the forward problem, in Section 3 we present a regularization approach for the proposed inverse problem, numerical examples are contained in Section 4.

2. Expansion of the forward solution

In this sections we present some definitions and derive an eigenfunction expansion of the forward solution u. Throughout the sequel of this article, we assume that q is continuously differentiable, w is continuous on $[a, b]$, and both positive, and that $f \in L^2(\Lambda_x \times \Lambda_t)$.

We use the notation $(\cdot, \cdot)_w$ to denote the weighted inner product on the space $L^2(\Lambda_x)$ which is defined by

$$(f, g)_w = \int_a^b w(x) f(x) g(x) dx,$$

with the induced norm $\|\cdot\|_w = \sqrt{(\cdot, \cdot)_w}$.

The Mittag-Leffler function of index (α, β) is the complex function defined as

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)},$$

where $\Gamma(\cdot)$ is the Euler's gamma function. For brevity, we write $E_\alpha(\cdot)$ to denote $E_{\alpha,1}(\cdot)$. We have the following result [1]:

Lemma 2.1. Let $\beta > 0$, then for $t > 0$ we have

$$\frac{d}{dt}\left[E_\alpha(-\beta t^\alpha)\right] = -\beta t^{\alpha-1} E_{\alpha,\alpha}(-\beta t^\alpha), \quad \alpha > 0.$$

Now we use the separation of variables technique to drive a series solution to (1.1)–(1.2). To this end, let λ_n, $n = 1, 2, \ldots$, be the eigenvalues of the Sturm-Liouville problem

$$-\frac{1}{w(x)}\frac{d}{dx}\left(q(x)\frac{dX}{dx}(x)\right) = \lambda X(x), \quad x \in \Lambda_x, \qquad X(a) = X(b) = 0, \tag{2.1}$$

with corresponding orthogonal eigenfunctions X_n, $n = 1, 2, \ldots$. We shall assume that the eigenfunctions have been normalized: $\|X_n\|_w = 1$ for all n. If u is sufficiently smooth, it can be expanded as

$$u(x,t) = \sum_{n=1}^{+\infty} T_n(t) X_n(x).$$

Plugging in this eigenfunction expansion in (1.1) then using the initial condition (1.2), we get

$$\frac{d^\alpha T_n}{dt^\alpha}(t) + \lambda_n T_n(t) = f_n(t), \quad T(0) = p_n, \tag{2.2}$$

where

$$f_n(t) = (f(\cdot,t), X_n)_w, \quad p_n = (p, X_n)_w.$$

From [2, Theorem 7.2], the solution of the fractional initial value problem (2.2) is given by

$$T_n(t) = p_n E_\alpha(-\lambda_n t^\alpha) + \int_0^t f_n(t-s) s^{\alpha-1} E_{\alpha,\alpha}(-\lambda_n s^\alpha) ds,$$

and consequently, a formal series solution to (1.1)–(1.2) is

$$u(x,t) = \sum_{n=1}^{+\infty} \left(p_n E_\alpha(-\lambda_n t^\alpha) + \int_0^t f_n(t-s) s^{\alpha-1} E_{\alpha,\alpha}(-\lambda_n s^\alpha) ds \right) X_n(x). \tag{2.3}$$

If the source term f depends on x only, then from Lemma 2.1 and simple manipulation the eigenfunction expansion (2.3) reduces to

$$u(x,t) = \sum_{n=1}^{+\infty} \left(p_n E_\alpha(-\lambda_n t^\alpha) + \lambda_n^{-1} f_n \left(1 - E_\alpha(-\lambda_n t^\alpha)\right)\right) X_n(x).$$

3. Regularization method

Now we introduce a regularization scheme for handling the backward problem which based on the eigenfunction expansion derived above.

Let $\overline{x}$ be the location of the measured data. Then from (2.3), we have

$$u(\overline{x},t) = \sum_{n=1}^{+\infty} \left(p_n E_\alpha(-\lambda_n t^\alpha) + \int_0^t f_n(t-s) s^{\alpha-1} E_{\alpha,\alpha}(-\lambda_n s^\alpha) ds \right) X_n(\overline{x}). \tag{3.1}$$

Since $\{X_n\}$ forms a complete orthonormal set in $L^2(\Lambda_x)$, we have the eigenfunction expansion

$$p(x) = \sum_{n=1}^{+\infty} p_n X_n(x),$$

provided $p \in L^2(\Lambda_x)$. To approximate the (Fourier) coefficients p_n (and hence p), we discretize equation (3.1) in time, truncate the infinite series, and replace the right-hand side by the measured (noisy) data u^m resulting in the equations

$$\sum_{j=1}^{N} \hat{p}_j \underbrace{E_\alpha(-\lambda_j t_i^\alpha) X_j(\overline{x})}_{a_{i,j}} = \underbrace{u^m(t_i) - \sum_{k=1}^{N} \left(\int_0^{t_i} f_k(t_i - s) s^{\alpha-1} E_{\alpha,\alpha}(-\lambda_k s^\alpha) ds \right) X_k(\overline{x})}_{b_i},$$

where $t_1 < t_2 < \cdots < t_M$ is a uniform partition of $\overline{\Lambda_t}$. This amounts to the system of linear equations

$$\mathbf{A}\hat{\mathbf{P}} = \mathbf{b} \tag{3.2}$$

where $\mathbf{A}_{i,j} = a_{i,j}$ and $\mathbf{b}_i = b_i$, $i = 1, \ldots, M$, $j = 1, \ldots, N$.

Since system (3.2) resulted in from discretizing an ill-posed problem, it is highly ill-conditioned. This means even if the error in the measured data is small, the error in the computed (least-square) solution is very large. A common remedy to this issue is regularization. We adopt the *Tikhonov regularization* method to solve (3.2). The resulted Tikhonov solution $\hat{\mathbf{P}}_\lambda$ is defined as the minimizer of optimization problem

$$\min_{\hat{\mathbf{P}} \in \mathbb{R}^N} \|\mathbf{A}\hat{\mathbf{P}} - \mathbf{b}\|_2^2 + \lambda^2 \|\hat{\mathbf{P}}\|_2^2, \tag{3.3}$$

where $\|\cdot\|_2$ stands for the standard Euclidean norm. The number $\lambda > 0$ is called the *regularization parameter* which controls the properties of the regularized solution; see Engl *et al.* [18] for more about regularization and the theory of ill-posed problems.

Choosing a good value of λ is vital in such type of analysis. A common strategy for choosing the value of λ is the *Generalized cross-validation* (GCV), which has been investigated by Wahba [19], and more recently by Hansen [20, 21] who gave the formulation of computations based on the singular value decomposition. It is an *a priori* method, which chooses the regularization parameter which minimizes the GCV function

$$G(\lambda) = \frac{\|\mathbf{A}\hat{\mathbf{P}}_\lambda - \mathbf{b}\|_2^2}{\left(\text{trace}\left(\mathbf{I}_M - \mathbf{A}\mathbf{A}^I\right)\right)^2},$$

where $\mathbf{I}_M$ is the $M \times M$ identity matrix, and A^I is a matrix which produces the regularized solution $\hat{\mathbf{P}}_\lambda$ when multiplied with $\mathbf{b}$, that is, $\hat{\mathbf{P}}_\lambda = \mathbf{A}^I \mathbf{b}$.

Finally, we let $\hat{\mathbf{P}}_\lambda = [\hat{p}_1 \ \hat{p}_2 \cdots \hat{p}_N]$ be the solution of the regularized problem (3.3), then the approximation to $p(x)$ is given by

$$\hat{p}_\lambda(x) = \sum_{n=1}^{N} \hat{p}_n X_n(x).$$

4. Numerical validation

Now we present numerical examples to test the feasibility and validity of the proposed algorithm.

In the experiments below, we take $M = 1000$ and $N = 10$, where as the observation location is taken to be $\overline{x} = 2^{-1/2}$ for the first example, and $\overline{x} = 3^{1/2}$ for the second.

For computing the regularization parameter as well as solving the optimization problem (3.3) we used the MATLAB code developed by Hansen [20, 21]. The MATLAB routine Podlubny [22] is used for fast evaluation of the Mittag-Leffler function.

We assume that the noisy data u^m is computed according to the formula

$$u^m(t_j) = u(\overline{x}, t_i) + \epsilon r_i, \quad i = 1, \ldots, M,$$

where ϵ represents the noise level, and r_i is a uniformly distributed random number in $[-1, 1]$.

To assess our approximations p_λ, we used the relative $L^2(\Lambda_x)$ error given by

$$\text{Relative Error} = \frac{\|p - p_\lambda\|_{L^2(\Lambda_x)}}{\|p\|_{L^2(\Lambda_x)}}.$$

Example 4.1. Consider the fractional heat equation

$$\begin{aligned} \frac{\partial^{2/3} u}{\partial t^{2/3}}(x,t) &= \frac{\partial^2 u}{\partial x^2}(x,t) + 45\pi^2 \sin(3\pi x), \;\; 0 < x < 1, \; 0 < t < 1, \\ u(x,0) &= 4\sin(2\pi x) + 5\sin(3\pi x), \;\; 0 < x < 1 \\ u(0,t) &= u(1,t) = 0, \;\; 0 < t < 1. \end{aligned}$$

The forward solution is given by

$$u(x,t) = 4E_{2/3}(-4\pi^2 t^{2/3})\sin(2\pi x) + 5\sin(3\pi x).$$

Here the eigenpairs for the Sturm-Liouville problem (2.1) are

$$\lambda_n = (n\pi)^2, \quad X_n(x) = \sqrt{2}\sin(n\pi x), \quad n = 1, 2, \ldots.$$

In Table 1 we compare the relative L^2-errors for several noise levels. The exact versus the recovered initial condition are shown in Figure 1. For this example, the condition number of the matrix $\mathbf{A}$ is 1.3×10^8 which is very large, reflecting the ill-posedness of the underlying inverse problem.

Example 4.2. In the second example, we take the fractional heat equation

$$\begin{aligned} \frac{\partial^{1/2} u}{\partial t^{1/2}}(x,t) &= x\frac{\partial}{\partial x}\left(x\frac{\partial u}{\partial x}(x,t)\right) + 1800\ln\left(\frac{2}{x}\right)^2 \ln(x), \;\; 1 < x < 2, \; 0 < t < 1, \\ u(x,0) &= \sin\left(\frac{5\pi \ln x}{\ln 2}\right) + g(x), \;\; 1 < x < 2 \\ u(1,t) &= u(2,t) = 0, \;\; 0 < t < 1. \end{aligned}$$

Table 1: Relative L^2 errors for Example 4.1.

Noise Level	**Relative Error**
10.0%	1.985E−01
1.0%	1.418E−01
0.1%	3.852E−02
0.01%	1.716E−02

Table 2: Relative L^2 errors for Example 4.2.

Noise Level	**Relative Error**
10.0%	1.726E−01
1.0%	1.142E−01
0.1%	4.571E−02
0.01%	1.024E−02

The forward solution is given by

$$u(x,t) = \exp\left(\left(\frac{5\pi}{\ln 2}\right)^4 t\right) \operatorname{erfc}\left(\left(\frac{5\pi}{\ln 2}\right)^2 \sqrt{t}\right) \sin\left(\frac{5\pi \ln x}{\ln 2}\right) + g(x),$$

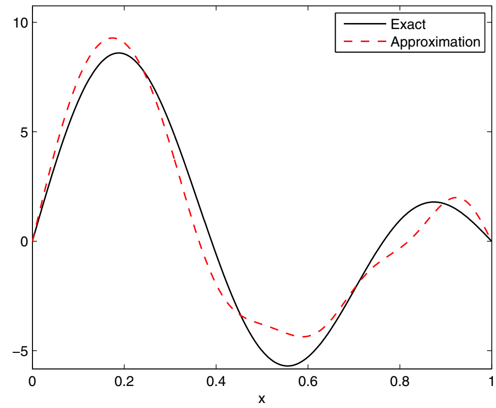
where $g(x) = 30\left(2\ln(2)^4 \ln(2/x) - 2\ln(2/x)^5 - 5\ln(2/x)^4 \ln(x)\right)$. The eigenpairs for (2.1) are

$$\lambda_n = \frac{n^2\pi^2}{(\ln 2)^2}, \quad X_n(x) = \sqrt{\frac{2}{\ln 2}} \sin\left(\frac{n\pi \ln x}{\ln 2}\right), \quad n = 1, 2, \ldots .$$

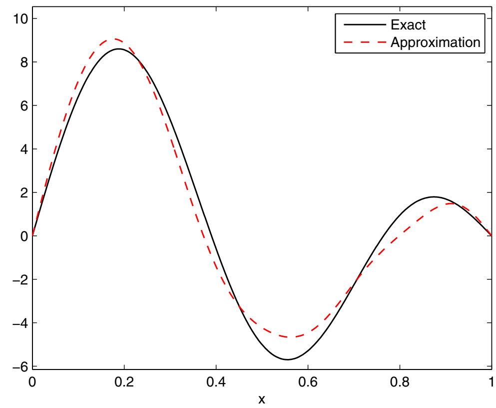
In Table 2 we compare the relative L^2-errors for several noise levels. The exact versus the recovered initial condition are shown in Figure 3. For this example, the condition number of the matrix $\mathbf{A}$ is 2.4×10^7.

5. Conclusions and future work

We investigated the possibility of recovering the initial distribution of a fractional heat equation from noisy interior data. We proposed a regularization scheme based on the



(a) $\epsilon = 10\%$

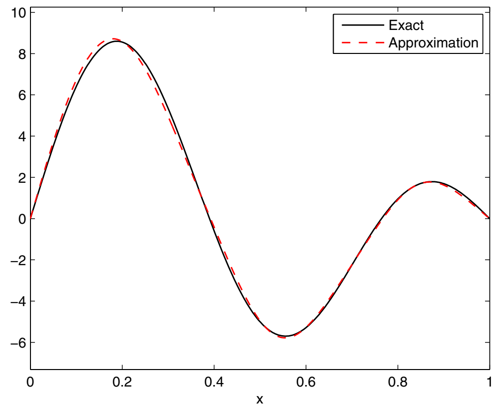


(b) $\epsilon = 1\%$

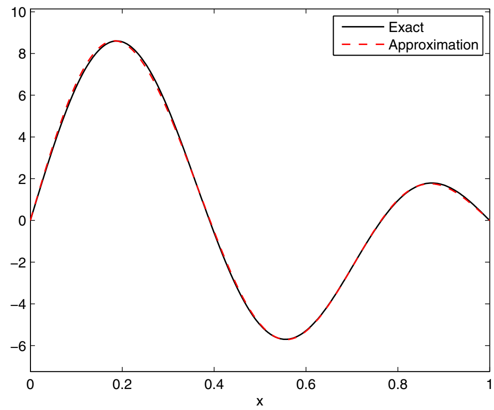
Figure 1: Exact and recovered initial condition for Example 4.1 with several noise levels ϵ.

eigenfunction expansion of the forward solution.

Our numerical experiments showed noteworthy results. However our analysis does not contain any convergence rates which we hope to obtain in a future work. Furthermore, we look to prove convergence results and give error bounds, which are of prominent importance for applied problems; we defer these investigations for a sequel to this paper.



(c) $\epsilon = 0.1\%$



(d) $\epsilon = 0.01\%$

Figure 1: Continued.

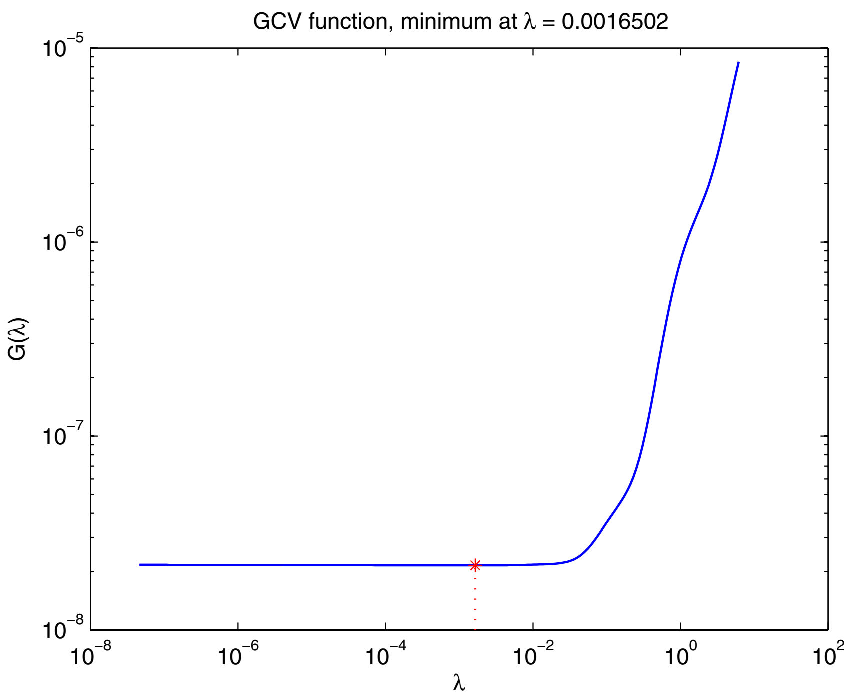
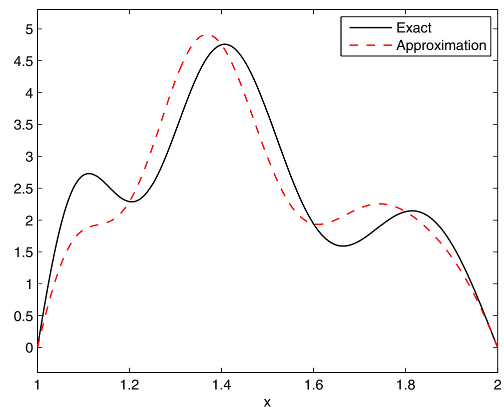


Figure 2: GCV function and its minimum for Example 4.1 corresponding to $\epsilon = 1\%$.



(a) $\epsilon = 10\%$

Figure 3: Exact and recovered initial condition for Example 4.2 with several noise levels ϵ.

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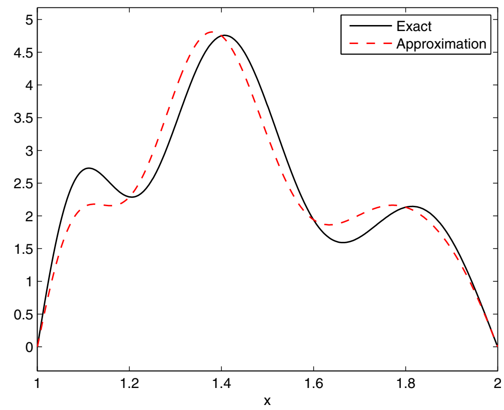
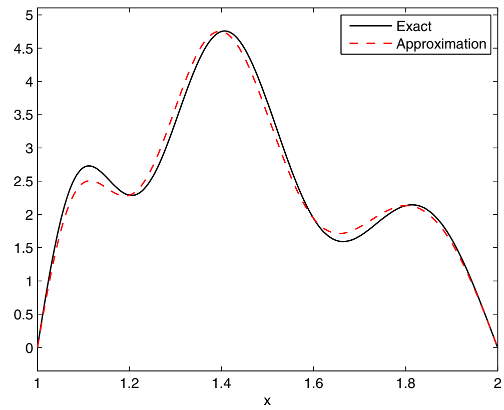


(b) $\epsilon = 1\%$



(c) $\epsilon = 0.1\%$

Figure 3: Continued.

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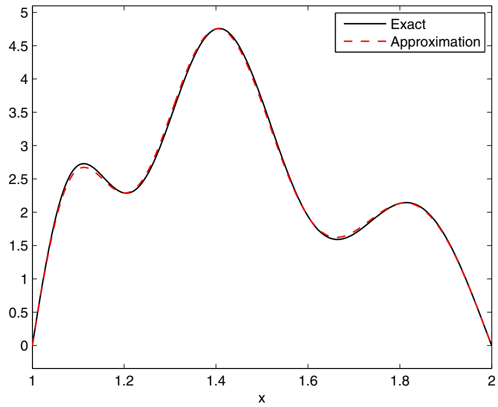

(d) $\epsilon = 0.01\%$

Figure 3: Continued.

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