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Numerical solution of the dynamic model of a chemical reactor by Hybrid functions

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Abstract

The dynamic model of chemical reactors can be transformed to a mixed Hammerstein integral equation. This paper present an efficient numerical procedure for solving the nonlinear Hammerstein integral equations of mixed type. Our method by use of a Hybrid function and some matrix properties of these functions convert these equations to an algebraic equation. These matrices are sparse so all calculation can be easily implemented. The reliability of the proposed scheme are demonstrated by numerical experiments.

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Keywords: Hammerstein integral equation of mixed type; Block-Pulse function; Hybrid function; Chemical reactor; The integration of cross product matrix.

1. Introduction

The theory and application of nonlinear integral equations is an important subject within applied mathematics [1-4]. Due to the fact that the nonlinear Hammerstein integral equations of mixed types appear in dynamic model of chemical reactor [1], we are interest in finding numerical solutions of these equations.

In this paper we are going to use hybrid Legendre and Block-Pulse as basis for the numerical solution of Hammerstein integral equations of mixed type that take the following form

$$u(x)=f(x)+\sum_{i=1}^{d}\int_0^1 k_i(x,s)\psi_i(s,u(s))ds, \quad 0\le x\le 1, \tag{1}$$

where f, u and $k_i, i=1,\dots,d$ are assume to be in L^2, with $\psi_i(x,u(x)), i=1,\dots,d$ nonlinear in u. We assume that Eq.(1) has a unique solution $u(x)$ to be determined. The existence results for these equations had been discussed in [2].

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2. Definition and some properties of hybrid functions of Block-Pulse and Legendre

2.1. Hybrid functions of Block-Pulse and Legendre

Consider the Legendre polynomials $L_m(x)$ on the interval $[-1,1]$:

$$L_0(x)=1,\quad L_1(x)=x,\quad L_{m+1}(x)=\frac{2m+1}{m+1}xL_m(x)-\frac{m}{m+1}L_{m-1}(x),\ m=1,2,3,...,$$

set $\{L_m(x):\ m=0,1,...\}$ in Hilbert space $L^2[-1,1]$ is a complete orthogonal set. A set of Block-Pulse functions $\phi_i(x), i=1,2,...,n$ and the orthogonal set of hybrid functions $h_{ij}(x), i=1,2,...,n, j=0,1,...,m-1$ that produces by Legendre polynomials and Block-Pulse functions on $[0,1)$ are defined as follows respectively:

$$\phi_i(x)=\begin{cases}1, & \frac{i-1}{n}\le x<\frac{i}{n},\\ 0, & \text{otherwise}\end{cases}\qquad h_{ij}(x)=\begin{cases}L_j(2nx-2i+1), & \frac{i-1}{n}\le x<\frac{i}{n},\\ 0, & \text{otherwise}\end{cases}$$

where n and m are the order of block-pulse functions and Legendre polynomials, respectively, and x is the normalized time.

2.2. function approximation

Any function $u(x)\in L^2[0,1)$ can be expanded in $u(x)=\sum_{i=1}^{\infty}\sum_{j=0}^{\infty}c_{ij}h_{ij}(x)$ where the hybrid coefficients are given by

$$c_{ij}=\frac{(u(x),h_{ij}(x))}{(h_{ij}(x),h_{ij}(x))},\quad i,j=1,2,...,\infty,$$

so that $(.,.)$ denotes the inner product. If $u(x)$ is piecewise constant or may be approximated as piecewise constant, then the sum may be terminated after nm terms, that is,

$$u(x)\simeq\sum_{i=1}^{n}\sum_{j=0}^{m-1}c_{ij}h_{ij}(x)=C^TB(x),$$

where

$$C=\left[c_{10},...,c_{1,m-1},c_{20},...,c_{2,m-1},...,c_{n0},...,c_{n,m-1}\right]^T, \tag{2}$$

$$B(x)=\left[h_{10}(x),...,h_{1,m-1}(x),h_{20}(x),...,h_{2,m-1}(x),...,h_{n0}(x),...,h_{n,m-1}(x)\right]^T. \tag{3}$$

We can also approximate the function $k(x,s)\in L^2([0,1)\times[0,1))$ as follows:

$$k(x,s)\simeq B^T(x)KB(s), \tag{4}$$

so that

$$K_{ij}=\frac{(B_i(x),(k(x,s),B_j(s)))}{(B_i(x),B_i(x))(B_j(s),B_j(s))},\quad i,j=1,2,...,nm.$$

2.3. The integration of the cross product

The integration of the cross product of two hybrid function vectors $B(x)$ can be obtained as [5]

$$D = \int_0^1 B(x)B^T(x)dx = \begin{bmatrix} L & 0 & \dots & 0 \\ 0 & L & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & L \end{bmatrix}, \tag{5}$$

where matrix L is a $m \times m$ diagonal matrix that is given by details in [5].

3. Numerical solvability of Hammerstein integral equation of mixed type

For solving Hammerstein integral equation of mixed type (1), we let

$$z_i(s) = \psi_i(s, u(s)), \quad 0 \le s \le 1, \tag{6}$$

then we get

$$u(x) = f(x) + \sum_{i=1}^{d} \int_0^1 k_i(x,s) z_i(s) ds. \tag{7}$$

substituting (7) in (6) results,

$$z_i(x) = \psi_i\left(x, f(x) + \sum_{i=1}^{d} \int_0^1 k_i(x,s) z_i(s) ds\right), \quad i = 1,2,\dots,d. \tag{8}$$

We approximate this equation as

$$z_i(x) \simeq \sum_{j=1}^{n} a_{i,j} B_j(x) = A_i^T B(x), \quad i = 1,2,\dots,d, \tag{9}$$

which $B(x)$ is defined with Eq.(3). Via Eqs.(4), (5), (8) and (9) we get

$$A_i^T B(x) = \psi_i\left(x, f(x) + \sum_{j=1}^{d} B^T(x) K_j D A_j\right), \quad i = 1,2,\dots,d. \tag{10}$$

In order to find $A_i, i =,1,2,\dots,d$ we collocate Eq.(10) in nm nodal points of Newton-Cotes as,

$$x_p = \frac{2p-1}{2nm}, \quad p = 1,2,\dots,nm. \tag{11}$$

Then we have Eq.(10) as following system of nonlinear equations

$$A_i^T B(x_p) = \psi_i\left(x_p, f(x_p) + \sum_{j=1}^{d} B^T(x_p) K_j D A_j\right), \quad p = 1,\dots,nm, \; i = 1,\dots,d. \tag{12}$$

This nonlinear system of equations can be solved by Newton's method. We used the Mathematica 7 software to solve this nonlinear system. After solving above nonlinear system we can achieve the unknown vectors $A_i, i = 1,2,\dots,d$. The required approximated solution $u(x)$ for our Hammerstein integral equation of mixed type (1), can be obtained by using Eqs.(7) and (9) as follows

$$u(x) = f(x) + \sum_{j=1}^{d} B^T(x) K_j D A_j. \tag{13}$$

4. Error estimation

If we approximate our function with Legendre polynomials, we have the following theorem for its error analysis.

Theorem 4.1: *Let* $u(x) \in H^K(-1,1)$ *(Sobolov space),* $u_J(x) = \sum_{i=0}^{J} a_i L_i(x)$ *be the best approximation polynomial of* $u(x)$ *in* L^2 *; then*

$$\left\| u(x) - u_J(x) \right\|_{L^2[-1,1]} \le C_0 J^{-k} \left\| u(x) \right\|_{H^k(-1,1)}, \tag{14}$$

where C_0 *is a positive constant, which depends on the selected norm and is independent of* $u(x)$ *and* J *; see [6,7].*

If we approximate our function with Hybrid Legendre and block-pulse functions, we have the following error bound for it accordingly.

Theorem 4.2: *Let* $u(x) \in H^K(0,1)$, $I_i = \left[\frac{i-1}{n}, \frac{i}{n}\right]$ *then*

$$\left\| u(x) - u_{nm}(x) \right\|_{L^2[0,1]} \le C_0 (nm)^{-k} \max_{0 \le i \le n} \left\| u(x) \right\|_{H^k(I_i)}, \tag{15}$$

Proof. By using Theorem 4.1, it is obvious.

Now we perform the estimating error for the Hammerstein integral equation of mixed type. If we approximate the answer of Eq.(1) by Eq.(13), we have:

$$e(x) = \left| u(x) - u_{nm}(x) \right| = \left| u(x) - f(x) - \sum_{j=1}^{d} I_j(x) \right|,$$

where $e(x)$ is defined as an error function and $I_j(x) = B^T(x) K_j D A_J$.

When we put $x = x_p$,

$$e(x_p) = \left| u(x_p) - f(x_p) - \sum_{j=1}^{d} I_j(x_p) \right|,$$

then our aim is: $e(x_p) \le 10^{-k_p}$ (k_p is any positive integer). If we prescribe $\max\left(10^{-k_p}\right) = 10^{-k}$ and whereas in our Hybrid function n and m are adjustable, for a fixed m we can increase n as far as the following inequality holds at each of the points x_p [5]:

$$e(x_p) \le 10^{-k}.$$

5. Numerical results

5.1. Example 1

Consider the nonlinear Hammerstein integral equation of mixed type with algebraic and exponential nonlinearity:

$$u(x) = f(x) + \sum_{i=1}^{2} \int_0^1 k_i(x,s) \psi_i(s, u(s)) ds, \tag{16}$$

where

$$f(x) = -\frac{x^4}{6} - \frac{x^6}{4} + \ln(x),$$
$$k_1(x,s) = x^4 s^4, \quad k_2(x,s) = x^6 s,$$
$$\psi_1(s, u(s)) = e^{u(s)}, \quad \psi_2(s, u(s)) = u^2(s),$$

and the exact solution is $u(x) = \ln(x)$. The computational results with $m = 4, n = 8$ and exact solutions with errors are shown in Table 1.

Table 1. Approximate solutions, exact solutions and absolute errors for Example 1.

x_i	Solution with $m=4, n=8$	Exact Solution	Absolute error $e(x_i)=\|u(x_i)-u_{nm}(x_i)\|$
0.0	$-\infty$	$-\infty$	0
0.1	-2.30258	-2.30258	0.0E-004
0.2	-1.60944	-1.60944	0.0E-004
0.3	-1.20397	-1.20397	0.0E-004
0.4	-0.91629	-0.91629	0.0E-004
0.5	-0.69316	-0.69315	0.1E-004
0.6	-0.51085	-0.51083	0.2E-004
0.7	-0.35676	-0.35667	0.9E-004
0.8	-0.22332	-0.22314	1.8E-004
0.9	-0.10570	-0.10536	3.4E-004
1.0	-0.00065	0	6.5E-004

6. Conclusion

In this paper the Hybrid Legendre and block-pulse functions and the associated integration of the cross product matrix used to solve Hammerstein integral equation of mixed type. The method is based upon reducing the equation into a set of algebraic equations. The main advantage of this method is its efficiency and simple applicability this truth that the values of n and m for this hybrid function are adjustable as well as being able to yield more accurate numerical solutions. The numerical example support this claim.

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