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Legendre collocation method and its convergence analysis for the numerical solutions of the conductor-like screening model for real solvents integral equation

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Abstract

In this paper, a reliable algorithm for solving the nonlinear Hammerstein integral equation arising from chemical phenomenon is presented. The conductor-like screening model for real solvents (COSMO-RS) integral equation will be solved by the shifted Legendre collocation method. This method approximates the unknown function with Legendre polynomials. The merits of this algorithm lie in the fact that, on the one hand, the problem will be reduced to a nonlinear system of algebraic equations. On the other hand, we show that the efficiency and accuracy of the shifted Legendre collocation method for solving these equations are remarkable. Also, this method is using a simple computational manner and its error analysis will be discussed by illustrating some theorems. Finally, two numerical experiments are given to confirm the superiority and efficiency of presented method with respect to some other well-known methods such as the Bernstein collocation method, Haar wavelet method and Sinc collocation method.

Keywords: Legendre polynomials, Hammerstein integral equations, Error analysis, numerical treatment, matrix equation.

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1 Introduction

In recent years, a number of methods have been proposed and applied successfully to obtain the approximate solution of various types of integral equations. It was found that the spectral methods are valid methods to obtain approximate solutions of integral equations [1–10]. In this paper, we apply the shifted Legendre collocation method (LCM) to solve COSMO-RS integral equation which was first presented in 1995 by A. Klamt [11]. The COSMO-RS model is a quantum chemistry the equilibrium thermodynamics method with the purpose of predicting chemical potential μ in liquids and is a novel approach for the description of salvation phenomena. In COSMO-RS calculations, the solute molecules are investigated in a virtual conductor environment. In such an environment, the solute molecule induces a polarization charge density σ on the interface between the molecule and the conductor. It processes the screening charge density σ on the surface of molecules to calculate the chemical potential μ of each species in solution. The stored COSMO results such as screening change density is used to calculate the chemical potential of the molecules in a liquid solvent or mixture in COSMO-RS [12]. Consider the following COSMO-RS integral equation [13]

$$\mu_S(\sigma) = -RT \ln \left[\int P_S(\sigma') \exp(-\frac{E_{int}(\sigma, \sigma') - \mu_S(\sigma')}{RT}) d\sigma' \right], \qquad (1)$$

where R is the gas constant, T is the temperature and the term $E_{int}(\sigma, \sigma')$ denotes the interaction energy expression for the segments with screening charge density σ and σ', respectively. The molecular interaction in solvent is $P_S(\sigma)$ and the chemical potential of the surface segments is described by $\mu_S(\sigma)$ which is to be determined. The σ-profile for the solvent of S, $P_S(\sigma)$, which might be a mixture of several compounds can be written by adding $P_S^i(\sigma)$ of the components weights by their mole fraction χ_i in mixtures by [14]:

$$P_S(\sigma) = \sum_{i}^{N} \chi_i P_S^i(\sigma).$$

The chemical potential of the surface segments is described $\mu_S(\delta)$ and should be determined. The domain of integration is determined by the characteristics of the σ-profile. The details of this model can be found in [11, 15, 16]. In [15], refinement and parameterization of this method was presented. In [17], Banerjee and Singh have used COSMO-RS to predict the vapor-liquid equilibria of ionic liquid systems. The performance of a COSMO-RS method in comparison to classical group contribution methods is presented in [18]. In [12, 19], Banerjee and Franke have demonstrated the accuracy and applicability of the COSMO-RS method.

Eq. (1) is the Hammerstein type nonlinear integral equations. There has been a notable interest in the numerical analysis of solutions of Hammerstein integral equations [20–27]. The Petrov-Galerkin, Galerkin, collocation, degenerate kernel and Nyström methods are most frequently used projection methods for solving the equations of this type [20, 28–34]. The classical method of successive approximation for Fredholm-Hammerstein integral equations was introduced in [35]. Brunner [36], applied a collocation-type method and Ordokhani [37] applied rationalized Haar function to nonlinear Volterra-Fredholm-Hammerstein integral equations. A variation of the Nyström method was presented in [38]. A collocation type method was developed in [38]. The asymptotic error expansion of a collocation type method for Volterra-Hammerstein integral equations has been considered in [39]. Maleknejad have used a numerical approach based on the Sinc quadrature which has exponential type convergence rate to solve Eq. (1) [13]. In [14], Eq. (1) has been solved by the Bernstein collocation method (BCM), Haar wavelet method (HWM), and Sinc collocation method (SCM).

In this work, we will extend the LCM to approximate the solution of Eq. (1). The properties of Legendre polynomials are used to reduce the problem into a system of algebraic equations. Besides, an estimation of the error bound for this method will be given. The obtained upper bound for the error indicates the convergence property of this algorithm. Finally, we apply this method to two numerical experiments in order to show the efficiency of presented method. These results confirm that the shifted Legendre collocation method is very effective and more accurate than BCM, HWM and SCM for solving COSMO-RS integral equation.

The rest of this paper is organized as follows. Preliminaries and notations needed hereafter are given in Section 2. In Section 3, the method for approximating the solution of Eq. (1) will be discussed. Section 4 is devoted to the convergence analysis of proposed method. Section 5 offers two numerical experiments to illustrate the efficiency of this algorithm. Finally, a brief conclusion is made in Section 6.

2 Preliminaries

The well-known Legendre polynomials are defined on the interval $[-1,\ 1]$ and can be determined with the aid of the following recurrence formula [40]

$$L_{i+1}(z) = \frac{2i+1}{i+1} z L_i(z) - \frac{i}{i+1} L_{i-1}(z), \quad i = 1,\ 2, ...,$$

where $L_0(z) = 1$ and $L_1(z) = z$. In order to use these polynomials on the interval $x \in [a, b]$, we define the so-called shifted Legendre polynomials by introducing the change of variable $z = \frac{2}{b-a}x - \frac{b+a}{b-a}$. Let the shifted Legendre polynomials $L_i(\frac{2}{b-a}x - \frac{b+a}{b-a})$ be denoted by $P_i(x)$. We consider the space $L^2[a, b]$ equipped with the following inner product and norm

$$\langle f, g\rangle = \int_a^b f(x)g(x)dx, \quad \|y\|_2 = \langle y, y\rangle^{\frac{1}{2}}.$$

The set of shifted Legendre polynomials forms a complete $L^2[a, b]$-orthogonal system such that the orthogonality condition is

$$\int_a^b P_i(x)\, P_j(x)\, dx = \begin{cases} \frac{b-a}{2i+1} & \text{for } i = j, \\ 0 & \text{for } i \neq j. \end{cases} \tag{2}$$

A function y(x), square integrable on $[a, b]$, may be expressed in terms of the shifted Legendre polynomials as

$$y(x) = \sum_{j=0}^{\infty} c_j P_j(x),$$

where the coefficients c_j are given by

$$c_j = \left(\frac{2}{b-a} j - \frac{b+a}{b-a}\right) \int_a^b y(x) P_j(x)\, dx, \quad j = 1,\ 2, ...$$

We consider the first $(N+1)-$terms of shifted Legendre polynomials. So we have

$$y(x) \simeq \sum_{j=0}^{N} c_j P_j(x) = C^T P(x), \tag{3}$$

where the shifted Legendre coefficient vector C and the shifted Legendre vector $P(x)$ are given by

$$C = [c_0, c_1, ..., c_N]^T, \tag{4}$$

and

$$P(x) = [P_0(x), P_1(x), ..., P_N(x)]^T. \tag{5}$$

3 Method of solution

In this section, an efficient method for approximating the solution of Eq. (1), by using the shifted Legendre polynomials will be illustrated.

Eq. (1), can be written as:

$$-\frac{\mu_S(\sigma)}{RT} = \ln\left[\int_a^b K(\sigma,\sigma')\exp\left(\frac{\mu_S(\sigma')}{RT}\right)d\sigma'\right], \tag{6}$$

where $K(\sigma,\sigma') = P_S(\sigma')\Omega(\sigma,\sigma')$ and $\Omega(\sigma,\sigma') = \exp\left(\frac{-E_{int}(\sigma,\sigma')}{RT}\right)$. Substituting $y(\sigma) = \exp\left(\frac{--\mu_S(\sigma)}{RT}\right)$ in Eq. (6), results in

$$y(\sigma) = \int_a^b K(\sigma,\sigma')(y(\sigma'))^{-1}d\sigma', \tag{7}$$

which is the well-known nonlinear Hammerstein integral equation. The general form of nonlinear Hammerstein integral equation is given by [41]

$$y(x) = g(x) + \int_a^b K(x,t)F(t,y(t))dt, \ a \le x \le b, \tag{8}$$

where $K(x,t)$, $g(x)$ and $F(t,y(t))$ are known functions and $y(x)$ is the unknown function which should be determined. In order to approximate the solution of Eq. (8), substituting relation (3) in Eq. (8), yields

$$C^T P(x) = g(x) + \int_a^b K(x,t)F(t,C^T P(t))dt, \tag{9}$$

where

$$F(t, C^T P(t)) = \frac{1}{C^T P(t)}.$$

Considering

$$A^TP(t) := F(t, C^TP(t)), \tag{10}$$

where

$$A = [a_0,\ a_1, ..., a_N]^T, \tag{11}$$

then, Eq. (9) can be rewritten as

$$C^TP(x) = g(x) + \int_a^b K(x,t)A^TP(t)dt. \tag{12}$$

Therefore,

$$C^TP(x) = g(x) + A^T\int_a^b K(x,t)P(t)dt. \tag{13}$$

Using Eqs. (10) and (13), we get

$$A^TP(x) = F\left(x, g(x) + A^T\int_a^b K(x,t)P(t)dt\right). \tag{14}$$

Collocating Eq. (14) at $N+1$ roots of the shifted Legendre polynomial $P_{N+1}(x)$, x_j, the following system of algebraic equations will be obtained

$$A^TP(x_j) = F\left(x_j, g(x_j) + A^T\int_a^b K(x_j,t)P(t)dt\right). \tag{15}$$

Through this system, the unknown coefficients A are determined and then using Eq. (10), C is resulted.

4 Convergence analysis

In this section, we will determin an estimation of the error bound for the approximate solution in the shifted Legendre collocation method for the nonlinear Hammerstein integral equation (8) on interval $[a,b]$. The existence and uniqueness of the solution of this equation are discussed by the Banach's fixed point theorem in [42] under the following assumptions:
(1) g is a continuous function on the interval $[a,b]$,
(2) K is a continuous function on the interval $[a,b]\times[a,b]$,
(3) F is a continuous function in the domain

$$W = \{t; a \le t \le b, |y| \le \infty\},$$

and satisfies the Lipschitz condition with respect to its two argument:

$$|F(x,y_1)-F(x,y_2)| \leq M\,|y_1-y_2|\,,$$

and

$$M_1 M(b-a) < 1,$$

where

$$M_1 = \max_{(x,t)\in[a,b]\times[a,b]} |K(x,t)|.$$

To discuss about the convergence analysis, at first we recall the following definitions.

Definition 1. *([43]) Function $q(x) \in P_n$ (the space of all polynomials of degree $\leq n$) is the best polynomial approximation for $f(x)$ on $[a,b]$ provided that $\|f-q\| \leq \|f-p\|, \quad \forall p \in P_n$.*

Definition 2. *([43]) A function $F(x,y)$ is said to satisfy in the Lipschitz condition if there is a constant $M>0$ such that $|F(x,y_1)-F(x,y_2)| \leq M\,|y_1-y_2|\,,$ for all y_1 and y_2 on $[a,b]$.*

Theorem 1. *Suppose that $\overline{y}(x)=\sum_{j=0}^{N}\overline{c}_j P_j(x)$ and $y_N(x)=\sum_{j=0}^{N} c_j P_j(x)$ are the best approximation and the approximate solution obtained by the proposed method, respectively. Then, we have*

$$\|\overline{y}-y_N\|_2 \leq \|\overline{C}-C\|_2 \left((b-a)\sum_{i=0}^{N}\frac{b-a}{2i+1}\right)^{\frac{1}{2}}, \tag{16}$$

where, the norm on the right hand side is the usual Euclidean norm for vectors,

$$\overline{C}=[\overline{c}_0,\overline{c}_1,...,\overline{c}_N]^T, \tag{17}$$

and

$$C=[c_0,c_1,...,c_N]^T. \tag{18}$$

Proof. The mentioned norm indicates that

$$\|\overline{y}-y_N\|_2 = \left(\int_a^b \left(\sum_{i=0}^{N}(\overline{c}_i-c_i)P_i(x)\right)^2 dx\right)^{\frac{1}{2}}. \tag{19}$$

Using the Holder's inequality, one obtains

$$\int_a^b \left(\sum_{i=0}^{N}(\overline{c}_i - c_i)P_i\left(x\right)\right)^2 dx \leq \int_a^b \left(\sum_{i=0}^{N}|\overline{c}_i - c_i|^2\right)\left(\sum_{i=0}^{N}|P_i\left(x\right)|^2\right)dx$$
$$= \left(\sum_{i=0}^{N}|\overline{c}_i - c_i|^2\right)\left(\sum_{i=0}^{N}\int_a^b |P_i\left(x\right)|^2 dx\right). \quad (20)$$

Considering relation (2), results in

$$\sum_{i=0}^{N}\int_a^b |P_i\left(x\right)|^2 dx = \sum_{i=0}^{N}\frac{b-a}{2i+1}. \quad (21)$$

Using relations (19), (20) and (21), we conclude that

$$\|\overline{y} - y_N\|_2 \leq \left(\sum_{i=0}^{N}|\overline{c}_i - c_i|^2\right)^{\frac{1}{2}}\left(\sum_{i=0}^{N}\frac{b-a}{2i+1}\right)^{\frac{1}{2}}$$
$$= \|\overline{C} - C\|_2\left((b-a)\sum_{i=0}^{N}\frac{1}{2i+1}\right)^{\frac{1}{2}}, \quad (22)$$

and the proof is completed. □

Theorem 2. *Considering the assumptions of Theorem 1 and the nonlinear Fredholm-Hammerstein integral equation (8), let*

$$K_1^2 = \int_a^b \left(\int_a^b |K(x,t)|^2\, dt\right) dx < \infty,$$

and $F\left(t, y(t)\right) \in C([a,b] \times R)$ satisfies the Lipschitz condition in the second variable. Then, the following result holds

$$\|y - y_N\|_2 \leq \frac{(b-a)^{\frac{1}{2}}\left(1 + K_1 C_1 (b-a)^{\frac{1}{2}}\right)\|\overline{C} - C\|_2\left(\sum_{i=0}^{N}\frac{1}{2i+1}\right)^{\frac{1}{2}}}{1-(b-a)^{\frac{1}{2}}K_1 C_1}, \quad (23)$$

where C_1 is the Lipschitz constant.

Proof. We can write the integral equation (8) as follows

$$g(x) = y(x) - \int_a^b K(x,t)F(t,y(t))dt. \tag{24}$$

Substituting $y_N(x)$ in this equation, results in

$$\widehat{g}(x) = y_N(x) - \int_a^b K(x,t)F(t,y_N(t))dt. \tag{25}$$

Also, since $\overline{y}(x)$ is the best approximate solution, we have

$$\overline{y}(x) = g(x) + \int_a^b K(x,t)F(t,\overline{y}(t))dt. \tag{26}$$

Subtracting Eqs. (24) from (25), we get

$$y(x) - y_N(x) = g(x) - \widehat{g}(x) + \int_a^b K(x,t)\left(F(t,y(t)) - F(t,y_N(t))\right)dt. \tag{27}$$

Let

$$u(x) = \int_a^b K(x,t)\left(F(t,y(t)) - F(t,y_N(t))\right)dt, \tag{28}$$

then, we can write

$$\|y - y_N\|_2 \leq \|g - \widehat{g}\|_2 + \|u\|_2. \tag{29}$$

If $K_1^2 = \int_a^b \left(\int_a^b |K(x,t)|^2\,dt\right)dx$, then according to the Holder's inequality, one obtains

$$\begin{aligned}
\|u\|_2^2 &= \int_a^b |u(x)|^2\,dx \\
&\leq \int_a^b \left(\int_a^b |K(x,t)||F(t,y(t)) - F(t,y_N(t))|dt\right)^2 dx \\
&\leq \int_a^b \left(\int_a^b |K(x,t)|^2\,dt\right)\left(\int_a^b |F(t,y(t)) - F(t,y_N(t))|^2\,dt\right)dx.
\end{aligned} \tag{30}$$

Using the Lipschitz condition, results in

$$|F(t,y(t)) - F(t,y_N(t))| \leq C_1|y(t) - y_N(t)|, \tag{31}$$

where $C_1 > 0$ is the Lipschitz constant. Substituting this bound in (30), one obtains

$$\begin{aligned}\|u\|_2^2 &\le K_1^2 \int_a^b \left(\int_a^b |F(t, y(t)) - F(t, y_N(t))|^2 \, dt \right) dx \\ &\le K_1^2 C_1^2 \int_a^b \left(\int_a^b |y(t) - y_N(t)|^2 \, dt \right) dx \\ &= K_1^2 C_1^2 \int_a^b \|y - y_N\|_2^2 dx \\ &= K_1^2 C_1^2 (b-a) \|y - y_N\|_2^2. \end{aligned} \tag{32}$$

Using (29) and (32), we have

$$\|y - y_N\|_2 \le \|g - \widehat{g}\|_2 + K_1 C_1 (b-a)^{\frac{1}{2}} \|y - y_N\|_2, \tag{33}$$

then,

$$\|y - y_N\|_2 \le \frac{\|g - \widehat{g}\|_2}{1 - (b-a)^{\frac{1}{2}} K_1 C_1}. \tag{34}$$

In order to find a bound on $\|g - \widehat{g}\|$, subtracting Eq. (25) from (26), we get

$$g(x) - \widehat{g}(x) = \overline{y}(x) - y_N(x) + \int_a^b K(x,t) \left(F(t, \overline{y}(t)) - F(t, y_N(t)) \right) dt. \tag{35}$$

Similarly, using the Lipschitz condition and the Holder's inequality, result in

$$\begin{aligned}\|g - \widehat{g}\|_2 &\le \|\overline{y} - y_N\|_2 + K_1 C_1 (b-a)^{\frac{1}{2}} \|\overline{y} - y_N\|_2 \\ &= (1 + K_1 C_1 (b-a)^{\frac{1}{2}}) \|\overline{y} - y_N\|_2, \end{aligned} \tag{36}$$

and from Theorem 1, one obtains

$$\begin{aligned}\|g - \widehat{g}\|_2 &\le \left(1 + K_1 C_1 (b-a)^{\frac{1}{2}}\right) \|\overline{C} - C\|_2 \left((b-a) \sum_{i=0}^{N} \frac{1}{2i+1} \right)^{\frac{1}{2}} \\ &= (b-a)^{\frac{1}{2}} \left(1 + K_1 C_1 (b-a)^{\frac{1}{2}}\right) \|\overline{C} - C\|_2 \left(\sum_{i=0}^{N} \frac{1}{2i+1} \right)^{\frac{1}{2}}. \end{aligned} \tag{37}$$

Substituting this bound in (34), results in

$$\|y-y_N\|_2 \leq \frac{(b-a)^{\frac{1}{2}}\,(1+K_1C_1(b-a)^{\frac{1}{2}})\|\overline{C}-C\|_2\left(\sum_{i=0}^{N}\frac{1}{2i+1}\right)^{\frac{1}{2}}}{1-(b-a)^{\frac{1}{2}}K_1C_1}. \qquad (38)$$

This completes the proof. □

5 Numerical experiments

In this section, two numerical experiments are given to demonstrate the capability of proposed method.

At the first experiment, consider the following COSMO-RS integral equation ([14])

$$y(\sigma)=\int_a^b P_S(\sigma')\Omega(\sigma,\sigma')(y(\sigma'))^{-1}d\sigma',$$

for a particular case of the energy expression, namely the electrostatic misfit energy. In this case, the relevant part of the kernel of integral equation is given by $\Omega(\sigma,\sigma')=\exp-(\sigma+\sigma')^2$ and the analytical function as synthetic σ-profile is

$$P_S(\sigma)=\begin{cases}\exp(-(5\sigma+2.5)^2)+\frac{1}{25\sigma^2+1}+\frac{(sin(5\sigma+2.5))^2}{(5\sigma-2.5)^2}+q(5\sigma), & -2\leq\sigma<2,\\ 0, & otherwise.\end{cases}$$

where $q(\sigma)=\begin{cases}-(\sigma-7)(\sigma-9), & 7\leq\sigma<9,\\ 0, & otherwise.\end{cases}$

So, COSMO-RS integral equations will be

$$y(\sigma)=\int_{-3}^{3} P_S(\sigma')\Omega(\sigma,\sigma')(y(\sigma'))^{-1}d\sigma'. \qquad (39)$$

Table 1 shows the numerical results which are obtained by our method and some other well-known methods such as BCM, HWM and SCM. In BPM, n terms have been applied in Bernstein series expansion and in HWM, the interval $[a,b]$ is divided into m equal subintervals, also the function $y(\sigma)$ expanded into m terms of Haar wavelet series. We see that our method are in a good agreement with those methods and even, we obtained these results with less amount of N.

Tab. 1: Numerical results for the first experiment.

	LCM				BCM			HWM			SCM		
x	$N=10$	$N=20$	$N=40$	$N=60$	$n=20$	$n=40$	$n=60$	$m=32$	$m=64$	$m=128$	$N=20$	$N=40$	$N=60$
-3	0.33987	0.33988	0.33985	0.33986	0.33983	0.3399	0.33989	0.44725	0.38618	0.3624	0.41505	0.31313	0.34715
-2.5	1.03931	1.03929	1.03829	1.03729	1.0436	1.03996	1.037	1.00784	1.0684	1.02392	1.25782	0.95974	1.0586
-2	1.99738	1.99737	1.968736	1.96736	1.9687	1.96368	1.96735	2.06715	1.94737	1.9819	2.36792	1.82947	2.00682
-1.5	2.39345	2.39343	2.39345	2.39345	2.39346	2.39354	2.39345	2.42834	2.39556	2.39436	2.84492	2.24043	2.43812
-1	2.04523	2.04521	2.04523	2.04523	2.0452	2.0453	2.04523	2.11768	2.0326	2.05572	2.36157	1.93929	2.07666
-0.5	1.49405	1.49405	1.49405	1.49405	1.49406	1.49409	1.49405	1.47893	1.51148	1.48742	1.62531	1.45005	1.50733
0	1.10484	1.10484	1.10484	1.10484	1.10484	1.10484	1.10484	1.04319	1.07366	1.08914	1.12284	1.09871	1.10684
0.5	0.76102	0.76102	0.76102	0.76102	0.76102	0.76102	0.76102	0.78163	0.74959	0.76651	0.74178	0.76831	0.75897
1	0.41419	0.41419	0.41419	0.41419	0.41419	0.41419	0.41419	0.39251	0.42374	0.40917	0.39492	0.42196	0.41195
1.5	0.16382	0.16382	0.16382	0.16382	0.16382	0.16381	0.16382	0.13146	0.14740	0.15548	0.15365	0.16812	0.16255
2	0.04623	0.04623	0.04623	0.04623	0.04623	0.04623	0.04623	0.05002	0.04415	0.04725	0.04255	0.04789	0.04572
2.5	0.00967	0.00967	0.00967	0.00967	0.00967	0.00967	0.00967	0.00860	0.01018	0.00942	0.00865	0.01019	0.00950
3	0.00163	0.00163	0.00163	0.00163	0.00163	0.00163	0.00163	0.03384	0.03375	0.03367	0.00140	0.00177	0.00158

At the second experiment, Consider the nonlinear Hammerstein integral equation ([14])

$$y(x) = g(x) + \int_a^b K(x,t)(y(t))^{-1}dt, \; a \le x \le b. \tag{40}$$

where $g(x) = \frac{21-11\exp(10)}{100}\exp(-10(1+x)) + \frac{1}{1+x}$, $K(x,t) = \exp(-10(x+t))$, $a = 0$ and $b = 1$. The exact solution of this equation is $y(x) = \frac{1}{1+x}$. We implement the suggested method with $N = 2$, $N = 5$ and $N = 8$. Tables 2, 3 and Figure 1 show the numerical results for the second experiment. Table 2 shows the absolute error $e_N(x) = |y(x) - y_N(x)|$ for the suggested method, where $y(x)$ and $y_N(x)$ are the exact and computed solution by our method, respectively. Also, this table compares these results with some other well-known methods such as BCM, HWM and SCM. These results confirm that the Legendre approximation method for solving this experiment is very effective and more accurate than BCM, HWM and SCM. In Table 3, one can see the values of $\|e_N\|_2 = \left(\int_0^1 e_N^2(x)dx\right)^{\frac{1}{2}}$, $\eta_N = \sum_{i=0}^N \left(\frac{1}{2i+1}\right)^{\frac{1}{2}}$ and $\|\overline{C} - C\|_2$. Also the value of K_1C_1 for this experiment is 0.0024. These show that the upper bound of the error is very small and near to $\|e_N\|_2$. The computing times (seconds) to obtain the numerical solution y_N are also given. In Figure 1, the numerical results by our method with $N = 2$, $N = 5$ and $N = 8$ are depicted. We see that, as N is increased, the error is decreased and also the error term $e_N(x)$ obtained by the proposed method is decreased as N is increased.

Tab. 2: Comparison of the absolute errors $e_N(x)$ for the second experiment.

x	LCM($N=8$)	BCM($n=10$)	HWM($m=32$)	SCM($N=10$)
0	1.454182e-18	0	0.0153187	0.00775417
0.1	1.895847e-17	2.22045e-16	0.00765666	0.0028526
0.2	1.136562e-17	3.33067e-16	0.0021544	0.00104941
0.3	2.793701e-19	3.33067e-16	0.00185752	0.000386057
0.4	3.115230e-19	1.11022e-16	0.00481696	0.000142023
0.5	7.577227e-19	0	0.00687241	0.0000522472
0.6	2.151335e-20	1.11022e-16	0.0036406	0.0000192207
0.7	2.729578e-19	1.11022e-16	0.00107926	7.07089e-6
0.8	2.425443e-20	1.11022e-16	0.00096621	2.60123e-6
0.9	0	0	0.00260984	9.56941e-7
1	0	0	0.00393701	3.52039e-7

Tab. 3: Numerical results for the second experiment.

N	$\|e_N\|_2$	η_N	$\|C'-C\|_2$	Computing time
2	1.38069e-16	1.23828	6.7514e-16	1.5346
5	3.20194e-17	1.37048	6.0263e-17	2.1561
8	6.10294e-19	1.44244	1.2604e-18	3.9649

6 Conclusion

In this paper, the shifted Legendre collocation method was applied to obtain the solution of COSMO-RS integral equations. The properties of Legendre polynomials were used to convert the integral equation into a system of algebraic equations which could be solved more easily. Also, the convergence property of our method for solving COSMO-RS integral equation has been discussed. We saw that the solutions could be more accurate by increasing N. The obtained results showed that the LCM for solving COSMO-RS integral equation was very effective with high accuracy in comparison with some other well-known methods such as BCM, HWM and SCM.

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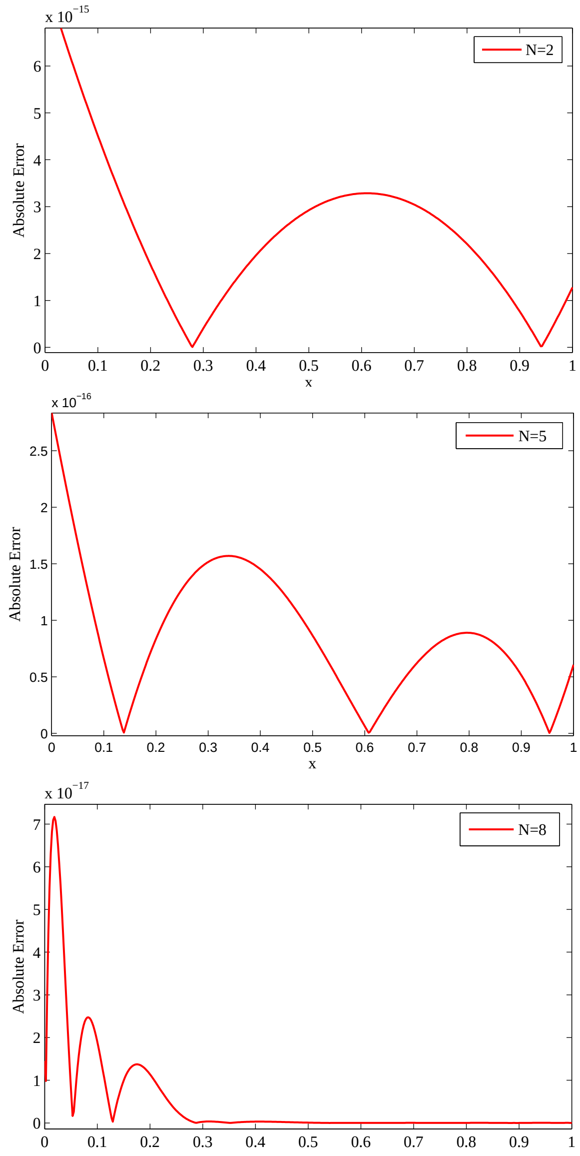

Fig. 1: Plot of the absolute error $e_N(x)$ with $N=2$, $N=5$ and $N=8$ for the second experiment.

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