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Optimized stochastic approach for integral equations

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***Abstract*—An optimized Monte Carlo approach (OPTIMIZED MC) for a Fredholm integral equations of the second kind is presented and discussed in the present paper. Numerical examples and results are discussed and MC algorithms with various initial and transition probabilities are compared.**

I. Introduction

INTEGRAL equations are of high importancy in various areas of applied mathematics [7]. That is why it is important to construct effective methods to solve integral equations. An important advantage of Monte Carlo (MC) methods is that they allow to search an unknown linear functional of the solution directly [1].

II. Formulation of the problem

The Fredholm integral equation of the second kind has been analyzed:

$$u\left(x\right)=\int_{\Omega}k\left(x,x'\right)u\left(x'\right)dx'+f\left(x\right)\ \ or\ u=\mathcal{K}u+f,\quad(1)$$

where

$$x,x'\in\Omega\subset\mathbb{R}^{d},\ u(x),f(x)\in L_{2}(\Omega),\ k(x,x')\in L_{2}(\Omega\times\Omega)$$

and $\mathcal{K}$ is the integral operator. Usually a linear functional from the solution:

$$J(u)=\int\varphi(x)u(x)dx=(\varphi,u)\qquad(2)$$

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should be evaluated in various problems. A MC algorithm is described below. Let $\varphi(x)\in L_{2}(\Omega)$. A set of permissible densities is defined:

$$\pi(x),\ p(x,x'):\ \pi\left(x\right)\geq0,\ p\left(x,x'\right)\geq0,$$

$$\int_{\Omega}\pi\left(x\right)dx=1,\int_{\Omega}p\left(x,x'\right)dx'=1,\ x\in\Omega\subset\mathbb{R}^{d}.$$

We define a Markov chain $T_{k}:\ x_{0}\rightarrow x_{1}\rightarrow\cdots\rightarrow x_{k}$ [4] with length k started from the initial state x_{0}. If the approximate initial solution coincides with the corresponding right-hand side $f(x)$, a MC algorithm for integral equations [6] is defined by:

$$E\theta_{k}[\varphi]=\left(\varphi,u^{(k)}\right),\ \theta_{k}[\varphi]=\frac{\varphi\left(x_{0}\right)}{\pi\left(x_{0}\right)}\sum_{j=0}^{k}W_{j}f\left(x_{j}\right),$$

$$W_{0}=1,\ W_{j}=W_{j-1}\frac{k(x_{j-1},x_{j})}{p(x_{j-1},x_{j})},\ j=1,\ldots,k,$$

$$\left(\varphi,u^{(k)}\right)\approx\frac{1}{N}\sum_{n=1}^{N}\theta_{k}[\varphi]_{n}.$$

III. A probabilistic error estimate

The probabilistic error is $r_{N}\leq0.6745\sigma\left(\theta\right)\frac{1}{\sqrt{N}}$ [3], [2], where N is the number of samples of the random variable θ and $\sigma\left(\theta\right)=\left(D\theta\right)^{1/2}$ is the standard deviation of the random variable θ for which $E\theta_{k}\left[\varphi\right]=\left(\varphi,u^{(k)}\right)=\sum_{j=0}^{k}(\varphi,\mathcal{K}^{(j)}f)$, where for point $x=(x_{0},\ldots,x_{j})\in G\equiv\Omega^{j+1}\subset\mathbb{R}^{d(j+1)},\ j=1,\ldots,k:$

$$(\varphi,\mathcal{K}^{(j)}f)=\int_{\Omega}\varphi(x_{0})\mathcal{K}^{(j)}f(x_{0})dx_{0}=$$

$$=\int_{G}\varphi(x_{0})k(x_{0},x_{1})\ldots k(x_{k-1},x_{j})f(x_{j})dx_{0}dx_{1}\ldots dx_{j}=$$

$$\int_G F(x)dx,$$

where

$$F(x) = \varphi(x_0)k(x_0,x_1)\dots k(x_{k-1},x_j)f(x_j),\ x \in G \subset \mathbb{R}^{d(j+1)}.$$

Using the inequality $D\sum_{j=0}^{k}\theta_k^{(j)} \leq \left(\sum_{j=0}^{k}\sqrt{D\theta_k^{(j)}}\right)^2$, and the variance properties we have the following inequalities [1]:

$$r_N \leq$$

$$\frac{0.6745}{\sqrt{N}}\sum_{j=0}^{k}\left(\int_G\left(\mathcal{K}^{(j)}\varphi f\right)^2 pdx - \left(\int_G \mathcal{K}^{(j)}\varphi f p dx\right)^2\right)^{1/2} \leq$$

$$\leq \frac{0.6745}{\sqrt{N}}\sum_{j=0}^{k}\left(\int_G\left(\mathcal{K}^{(j)}\varphi f\right)^2 pdx\right)^{1/2}$$

$$= \frac{0.6745}{\sqrt{N}}\|\varphi\|_{L_2}\|f\|_{L_2}\sum_{j=0}^{k}\left\|\mathcal{K}^{(j)}\right\|_{L_2}.$$

The following estimate is obtained:

$$r_N \leq \frac{0.6745\|f\|_{L_2}\|\varphi\|_{L_2}}{\sqrt{N}\left(1-\|\mathcal{K}\|_{L_2}\right)}.$$

IV. A SYSTEMATIC ERROR ESTIMATE

The sequence [2] $u^{(1)},\ u^{(2)},\dots$ is defined by the recursion formula $u^{(k)} = \mathcal{K}u^{(k-1)}+f, k = 1,2,\dots$. The formal solution of the equation (1) is the truncated Neumann series $u^{(k)} = f+\mathcal{K}f+\dots+\mathcal{K}^{(k-1)}f+\mathcal{K}^{(k)}u^{(0)}, k>0$, where the k^{th} iteration of $\mathcal{K}$ is denoted by $\mathcal{K}^{(k)}$, and $u^{(k)} = \sum_{i=0}^{k-1}\mathcal{K}^{(i)}f + \mathcal{K}^{(k)}u^{(0)}$.

We construct the k - residual vector of the systematic error $r^{(k)}$: $r^{(k)} = f-(I-\mathcal{K})u^{(k)} = (I-\mathcal{K})\left(u-u^{(k)}\right)$.

By the definition of $r^{(k)}$: $r^{(k)} = f-u^{(k)}+\mathcal{K}u^{(k)} = u^{(k+1)}-u^{(k)}$ and $r^{(k+1)} = u^{(k+2)}-u^{(k+1)} = \mathcal{K}u^{(k+1)}+f-\mathcal{K}u^{(k)}-f = \mathcal{K}\left(u^{(k+1)}-u^{(k)}\right) = \mathcal{K}r^{(k)}$.

We have $r^{(0)} = u^{(1)}-u^{(0)} = \mathcal{K}u^{(0)}+f-u^{(0)} = \mathcal{K}f$, $r^{(k+1)} = \mathcal{K}r^{(k)} = \mathcal{K}^{(2)}r^{(k-1)} = \dots = \mathcal{K}^{(k+1)}r^{(0)}$.

So we obtain $u^{(k+1)} = u^{(k)}+r^{(k)} = u^{(k-1)}+r^{(k-1)}+r^{(k)} = \dots = u^{(0)}+r^{(0)}+\dots+r^{(k)} = u^{(0)}+r^{(0)}+\mathcal{K}r^{(0)}+\mathcal{K}^{(2)}r^{(0)}+\dots+\mathcal{K}^{(k)}r^{(0)} = u^{(0)}+\left(I+\mathcal{K}+\dots+\mathcal{K}^{(k)}\right)r^{(0)}$ [4].

If $\|\mathcal{K}\|_{L_2} < 1$ then the Neumann series $u = \sum_{i=0}^{\infty}\mathcal{K}^{(i)}f$ is convergent and $u^{(k+1)} \xrightarrow{k\to\infty} u$ therefore from $u^{(k+1)} = u^{(0)}+\left(I+\mathcal{K}+\dots+\mathcal{K}^{(k)}\right)r^{(0)}$ and $k\to\infty$ we have $u = u^{(0)}+(I-\mathcal{K})^{-1}r^{(0)}$. After simple transformations $u = \mathcal{K}u+f = \mathcal{K}u^{(0)}+\mathcal{K}(I-\mathcal{K})^{-1}r^{(0)}+f = u^{(1)}+\mathcal{K}(I-\mathcal{K})^{-1}r^{(0)}$.

Doing this k times we obtain: $u = u^{(k)}+\mathcal{K}^{(k)}(I-\mathcal{K})^{-1}r^{(0)}$. The following inequalities are established applying the Cauchy-Schwarz inequality:

$$r^{(k)} = \left\|u-u^{(k)}\right\|_{L_2} \leq$$

$$\frac{\|\mathcal{K}\|_{L_2}^k\left\|r^{(0)}\right\|_{L_2}}{1-\|\mathcal{K}\|_{L_2}} \leq \frac{\|\mathcal{K}\|_{L_2}^k\|f\|_{L_2}\|\mathcal{K}\|_{L_2}}{1-\|\mathcal{K}\|_{L_2}} =$$

$$\frac{\|\mathcal{K}\|_{L_2}^{k+1}\|f\|_{L_2}}{1-\|\mathcal{K}\|_{L_2}}.$$

The systematic error is estimated in following way:

$$\left|(\varphi,u)-\left(\varphi,u^{(k)}\right)\right| \leq \|\varphi\|_{L_2}\left\|u-u^{(k)}\right\|_{L_2} \leq$$

$$\frac{\|\varphi\|_{L_2}\|f\|_{L_2}\|\mathcal{K}\|_{L_2}^{k+1}}{1-\|\mathcal{K}\|_{L_2}}.$$

V. THE OPTIMIZED STOCHASTIC APPROACH

Let us denote by δ an accuracy to solve the task under consideration (2). This means that:

$$r_N \leq \frac{0.6745\|\varphi\|_{L_2}\|f\|_{L_2}}{\sqrt{N}\left(1-\|\mathcal{K}\|_{L_2}\right)} \leq \frac{\delta}{2},$$

$$r_k \leq \frac{\|\varphi\|_{L_2}\|f\|_{L_2}\|\mathcal{K}\|_{L_2}^{k+1}}{1-\|\mathcal{K}\|_{L_2}} \leq \frac{\delta}{2}.$$

For a Fredholm integral equation (1) the lower bounds for N and k for the OPTIMIZED MC algorithm are:

$$N \geq \left(\frac{1.349\|\varphi\|_{L_2}\|f\|_{L_2}}{\delta\left(1-\|\mathcal{K}\|_{L_2}\right)}\right)^2,\ k \geq \frac{\ln\frac{\delta\left(1-\|\mathcal{K}\|_{L_2}\right)}{2\|\varphi\|_{L_2}\|f\|_{L_2}\|\mathcal{K}\|_{L_2}}}{\ln\|\mathcal{K}\|_{L_2}}.$$

We have also obtained an optimal ratio between k and N: For a Fredholm integral equation (1) the lower bounds for N and k for the OPTIMIZED MC algorithm are:

$$N \geq \left(\frac{1.349\|\varphi\|_{L_2}\|f\|_{L_2}}{\delta\left(1-\|\mathcal{K}\|_{L_2}\right)}\right)^2,\ k \geq \frac{\ln\frac{0.6745}{\|\mathcal{K}\|_{L_2}\sqrt{N}}}{\ln\|\mathcal{K}\|_{L_2}}.$$

VI. NUMERICAL EXAMPLES AND RESULTS

A. Example 1

The first example is:

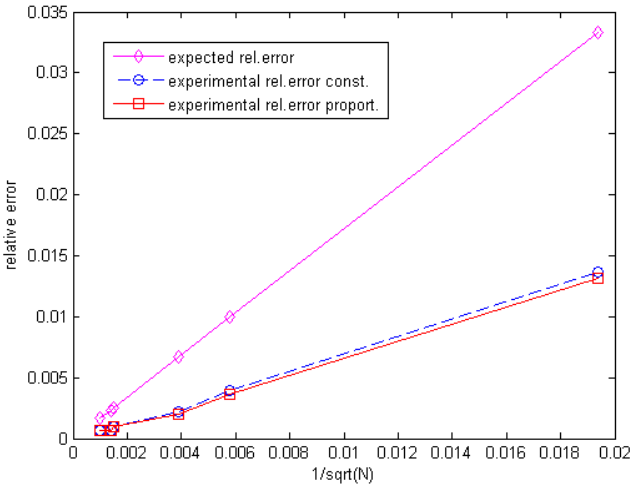
$$u(x) = \int_\Omega k(x,x')u(x')\,dx' + f(x),$$

$\Omega \equiv [0,1]$, $k(x,x') = \frac{1}{6}e^{x+x'}$, $f(x) = 6x-e^x$. $\varphi(x)$ is the delta function ($\Delta(x)$). The exact solution is $u(x) = 6x$. We are interested in the value of the solution at the middle of the interval. Firstly, the L_2 norms are computed: $\|\varphi\|_{L_2} = 1$, $\|\mathcal{K}\|_{L_2} = 0.5324$, $\|f\|_{L_2} = 1.7873$. For this example the exact solution is 3 and $\pi(x) = \Delta(x)$. We make 20 algorithm runs on Intel Core i5-2410M @ 2.3 GHz.

TABLE I
RESULTS FOR THE FIRST EXAMPLE.

δ	N	k	expected rel. error	BASIC rel. error	time (sec.)	OPTIMIZED rel. error	time (sec.)
0.1	2659	6	0.0333	0.0137	11	0.0132	5
0.03	29542	8	0.01	0.0039	62	0.0036	42
0.02	66468	9	0.0067	0.0022	140	0.0020	70
0.0075	472659	10	0.0025	0.001	1167	9.3671e-04	529
0.007	542593	11	0.00233	6.9639e-04	1562	6.3582e-04	614
0.005	1063482	11	0.00167	6.4221e-04	4412	6.2479e-04	2202

Fig. 1. Experimental and expected relative error.



B. Numerical results for the first example

The first two columns with the expected relative error (RE) and the computational time (CPU time) measured in seconds are for the case when the transition probabilities are constant functions (this is the standard MC method and we use the notation BASIC) and the last two columns are for the case when OPTIMIZED is used (this is also called the almost optimal MC algorithm). From the Tables it leads that the OPTIMIZED method gives better results (smaller relative errors and significantly smaller computational times).

We can see the comparison between the expected and experimental relative error on Figure 1 which shows that experimental RE confirms the expected RE.

The OPTIMIZED MC algorithm has a higher computational efficiency than the BASIC MC algorithm because its CPU time is smaller.

C. Example 2

The next example is a biology analytically tractable model [5]:

TABLE II
RESULTS FOR THE SECOND EXAMPLE.

δ	N	k	expected rel. error	BASIC rel. error	time sec.	OPTIMIZED rel. error	time sec.
0.23	132	3	0.1395	0.0123	0.5	0.0121	0.2
0.037	5101	4	0.0224	0.0041	11	0.0040	7
0.025	11172	5	0.0152	0.0014	16	0.0012	9
0.014	35623	6	0.0085	4.5725e-04	56	4.0010e-04	34
0.0055	230809	7	0.0033	1.5242e-04	424	9.8811e-05	346
0.0045	344788	7	0.0027	1.5242e-04	605	1.4893e-04	592

$$u(x) = \int_{\Omega} k(x, x') u(x')\, dx' + f(x),$$

$\Omega \equiv [0,1]$, $k(x,x') = \frac{1}{3}e^x$, $f(x) = \frac{2}{3}e^x$. $\varphi(x)$ is the delta function. The exact solution is $u(x) = e^x$. We are interested in the value of the solution at the middle point of the interval. The L_2 norms are evaluated as follows: $\|\varphi\|_{L_2} = 1$, $\|\mathcal{K}\|_{L_2} = 0.3917$, $\|f\|_{L_2} = 1.1915$. Here the exact solution is 1.6487 and $\pi(x) = \Delta(x)$. We make 20 algorithm runs on the same computational unit.

D. Numerical results for the second example

One can see that the OPTIMIZED method gives slightly better results than the BASIC MC and the results are closer when the initial probability is the delta function. However again the OPTIMIZED MC algorithm has a higher computational efficiency than the BASIC algorithm because its CPU time is shorter.

E. Example 3

We study the following example describes the procedure of teaching of neural networks [4], [5]:

$$u(x) = \int_{\Omega} k(x, x') u(x')\, dx' + f(x),$$

$\Omega \equiv [-2,2]$, $k(x,x') = \frac{0.055}{1+e^{-3x}} + 0.07$, $f(x) = 0.02\left(3x^2 + e^{-0.35x}\right)$, $\varphi(x) = 0.7((x+1)^2\cos(5x) + 20)$.

Here $\varphi(x) = 0.7((x+1)^2 \cos 5x + 20)$. The exact solution is 8.98635750518 [2]. We calculate: $\|\varphi\|_{L_2} = 27.7782$, $\|\mathcal{K}\|_{L_2} = 0.2001$, $\|f\|_{L_2} = 0.2510$.
We make 20 algorithm runs on the same processor.

F. Numerical results for the third example

The results presented in Table III demonstrates that the OPTIMIZED MC method gives much smaller relative errors than the BASIC MC algorithm for larger values of N and k. In the case of smaller values of these quantities the BASIC MC gives smaller relative errors, but the RE obtained with OPTIMIZED method are closer to the expected RE. Using the OPTIMIZED approach we see that the experimental RE confirms the expected RE. We also see that in the OPTIMIZED algorithm is a little bit slower because we use the acceptance-rejection method for modeling the initial probabilities.

TABLE III
RESULTS FOR THE THIRD EXAMPLE.

δ	N	k	expected rel. error	BASIC rel. error	time sec.	OPTIMIZED rel. error	time sec.
0.4	865	3	0.0445	0.0052	3	0.0239	5
0.2	3457	4	0.0223	0.0094	9	0.0121	23
0.1	13827	4	0.0111	0.0113	28	0.0086	46
0.05	55306	5	0.00556	0.0177	132	0.0032	222
0.028	176357	5	0.00312	0.0176	448	0.0031	540
0.02	345659	6	0.00233	0.0202	901	0.0013	1090

VII. CONCLUSION

In this paper we present an optimized stochastic algorithm for solving the Fredholm integral equation of the second kind. Two main cases are taken into account - the initial probability coincides with the delta function, and the second case when the initial probability is different from the delta function. The results from the numerical tests in the first case show that the OPTIMIZED MC reaches much smaller computational times than the BASIC MC with constant probabilities and comparable relative errors respectively. The results from the numerical tests in the second case show that the OPTIMIZED MC reaches much smaller relative errors than the BASIC MC with constant probabilities and comparable computational times respectively. the OPTIMIZED MC has a higher computational efficiency than the BASIC MC. The main conclusion here is that the OPTIMIZED MC approach is characterized by a higher computational efficiency (proportional to relative error and compuatational time) in both cases under consideration.

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