

## A PROGRAM FOR SOLVING FIRST KIND FREDHOLM INTEGRAL EQUATIONS BY MEANS OF REGULARIZATION

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Received 5 February 1985

### PROGRAM SUMMARY

*Title of program:* FIREGU

*Catalogue number:* AABX

*Program obtainable from:* CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue)

*Computer:* CDC CYBER 175-750; *Installation:* SARA (Academic Computer Centre Amsterdam)

*Operating system:* NOS/BE

*Programming language:* FORTRAN 77

*Program Library used:* NAG FORTRAN LIBRARY, MARK 10 (SUBROUTINE F04ASF; this, in turn, uses other NAG routines)

*Programming language:* FORTRAN 77

*High speed storage requested:* 60 K

*No. of bits in a word:* 60

*Peripheral used:* line printer

*No. of lines in combined program and test deck:* 321

*Keywords:* Fredholm integral equation of the first kind, regularization, elastic electron-atom scattering, dispersion relation

#### *Nature of the physical problem*

Fredholm integral equations of the first kind arise in the mathematical analysis of many physical problems (cf. Nedelkov [1]). An important characteristic of such problems is that the information which we seek about a physical quantity  $A$  can only be obtained *indirectly*, by measuring some other quantity  $B$  which has some connection with  $A$ . Often, this connection can be expressed mathematically in terms of a Fredholm first kind integral equation.

#### *Method of solution*

The first kind Fredholm integral equation is solved by means of the regularization method of Tihonov [2,3] and Phillips [4].

#### *Running time*

Approximately proportional to the third power of the number of data points.

#### *References*

- [1] I.P. Nedelkov, *Comput. Phys. Commun.* 4 (1972) 157.
- [2] A.N. Tihonov, *Soviet Math. Dokl.* 4 (1963) 1035, 1624.
- [3] A.N. Tihonov and V.Y. Arsenin, *Solution of Ill-posed Problems* (Winston, Washington, DC, 1977).
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## LONG WRITE-UP

### 1. Introduction

The linear first kind Fredholm integral equation

$$\int_a^b K(x, y)f(y)dy = g(x), \quad c \leq x \leq d, \quad (1.1)$$

where  $f$  is the unknown function, and  $g$  and  $K$  are given functions, arises in the mathematical analysis of problems from many branches of physics, chemistry and biology [3]. Also several classical mathematical problems, like the problem of harmonic continuation, numerical inversion of the Laplace transform, the backwards heat equation, and numerical differentiation, can be formulated as equations of the form (1.1).

We assume that  $f$  and  $g$  are elements of certain linear spaces  $F$  and  $G$ , respectively. Defining the linear operator  $\mathcal{K}: F \rightarrow G$  by  $(\mathcal{K}f)(x) := \int_a^b K(x, y)f(y)dy$ , we write (1.1) in operator notation as:

$$\mathcal{K}f = g, \quad g \in G \text{ given, } f \in F \text{ sought.} \quad (1.2)$$

In general, numerical solution of (1.1) is difficult, because (1.1) belongs to the class of so-called *ill-posed*, or *improperly posed* problems. The problem (1.2) is ill-posed (in the sense of Hadamard, cf. ref. [2]) if at least one of the following three assertions is *false* ( $F$  and  $G$  are assumed to be complete metric spaces):

- (i) for every  $g \in G$  there exists a solution  $f \in F$ ;
- (ii) the solution of (1.2) is unique;
- (iii) the solution of (1.2) depends continuously on the data  $g$ .

Note that this definition depends on the spaces  $F$  and  $G$ . A problem may be ill-posed with respect to given  $F$  and  $G$ , but well-posed in other metrics. In general, (1.2) is ill-posed because the solution  $f$  of (1.2) does not depend continuously on the data function  $g$ . This may be explained, at least heuristically, as follows. If  $K$  is a smooth function, then  $\mathcal{K}$  is a smoothing operator and small perturbations in  $g$  may be caused by large perturbations in  $f$ , which were smoothed down by  $\mathcal{K}$ .

In practical situations, the data function  $g$  is often the output of some measuring process, so that it is only approximately known in some dis-

crete set of points  $x_i \in [c, d]$ . Consequently, rather than (1.2) it is more realistic to consider the problem.

$$\mathcal{K}f = \tilde{g}, \quad (1.3)$$

where only  $\tilde{g}$  and  $\epsilon$  are known such that  $\|\tilde{g} - g\| \leq \epsilon$  for some norm  $\|\cdot\|$ . This may cause  $\tilde{g}$  to lie outside the range of the operator  $\mathcal{K}$ , so that there may not exist a solution of (1.3).

### 2. The regularization method

A survey of numerical methods for solving (1.1)–(1.3) may be found in refs. [5,11]. Here, we describe a simple implementation of the so-called *regularization* method of Phillips [4] and Tihonov [9–11]. This method essentially consists of the replacement of the ill-posed problem (1.3) by the well-posed problem (i.e. for which the three assertions (i), (ii) and (iii) above are *true*):

Minimize the quadratic functional  $\phi_\alpha(f)$ , defined by

$$\phi_\alpha(f) := \|\mathcal{K}f - \tilde{g}\|^2 + \alpha \|Lf\|^2, \quad (2.1)$$

over all functions  $f$  in the compact set:

$$\{f: \|\mathcal{K}f - \tilde{g}\| \leq \epsilon\}.$$

Here,  $\alpha$  is a fixed positive number, the so-called *regularization parameter* and  $L$  is some linear operator, e.g.  $Lf = f$ ,  $f'$  or  $f''$ , or  $Lf = f - \hat{f}$  if an a priori approximation  $\hat{f}$  of  $f$  can be provided. If  $Lf$  is the  $i$ th derivative of  $f$ , then it is customary to speak about  *$i$ th order regularization*.

Under certain, mild conditions, (2.1) has a unique solution, which will be denoted by  $f_\alpha$ . Moreover,  $f_\alpha$  will converge as  $\epsilon \rightarrow 0$ , uniformly on  $[a, b]$ , to the solution of the equation  $\mathcal{K}f = g$  (if it exists), provided that  $\alpha$  satisfies

$$C_1\epsilon^2 < \alpha < C_2\epsilon^2 \quad (2.2)$$

for positive numbers  $C_1$  and  $C_2$ . Unfortunately,  $g$  is not known exactly and the ill-posedness of (1.3) will, generally, cause the solution  $f_\alpha$  of (2.1) to oscillate very wildly around the solution of the equation  $\mathcal{K}f = g$ , when  $\alpha$  is chosen to be close to



heading of this subroutine reads as follows:

SUBROUTINE FIREGU (KERNEL, N, X, G,  
Y, ALFA, LINFUN, F, RES)  
EXTERNAL KERNEL  
REAL KERNEL, X(N), G(N), Y(0:N), RES(6)

The parameters of FIREGU are:

**KERNEL:** a user-supplied external function which delivers the value of the kernel function  $K$  in the point  $(x, y)$  for any  $x$  in the interval  $[c, d]$  and any  $y$  in the interval  $[a, b]$ ;

**N:** the number of data points for which  $g$  is given and for which approximations to  $f$  are to be found; the maximum number allowed is 64;

**X(N), G(N):** arrays containing, on entry, the abscissae  $x_1, \dots, x_N$  and the corresponding data values  $g_1, \dots, g_N$ ;

**Y(0:N):** array of length  $N + 1$  containing, on entry, a subdivision of  $[a, b]$ ;

**ALFA** the regularization parameter, to be supplied by the user;

**LINFUN:** with this parameter, the user monitors the choice of the linear functional  $L$ :  
LINFUN = 1:  $Lf = f - \hat{f}$ ,  
= 2:  $Lf = f'$ ,  
= 3:  $Lf = f''$ ;

**F(N)** array of length  $N$  which, on exit, contains approximations to the solution  $f$  in the midpoints  $\bar{y}_j$ ; if LINFUN = 1 then, on entry, the user must provide in F an a priori estimate of the solution in these midpoints;

**RES(6)** array containing, on exit, the following information: ( $\|\cdot\|$  is the discrete  $L_2$ -norm)  
RES (1) =  $\|f - \hat{f}\|$ ,  
RES (2) =  $\|f'\|$ ,  
RES (3) =  $\|f''\|$ ,  
RES (4) =  $\|Kf - g\|$ ,  
RES (5) = minimum absolute value of the components of  $Kf - g$ ,  
RES (6) = maximum absolute value of the components of  $Kf - g$ .

## 5. Workspace

FIREGU uses 8448 words blank common workspace to be declared in the main program as follows:

COMMON K (64, 64), MAT (64, 64), RHS (64),  
WK1 (64), WK2 (64), FH (64)  
REAL K, MAT, RHS, WK1, WK2, FH

## 6. Test-examples

The subroutine FIREGU has been tested on the following problem with known solution:

$$K(x, y) = (x + y)^{-1}, \quad g(x) = x^{-1} \ln \left[ \frac{1 + x/a}{1 + x/b} \right],$$

$$f(y) = y^{-1},$$

$$[a, b] = [c, d] = [1, 5], \quad N = 16, 32,$$

$$x_i = 1 + (i - 1) * h_1,$$

$$i = 1, 2, \dots, N, \quad h_1 = 4/(N - 1), \quad (6.1)$$

$$y_i = 1 + i * h_2, \quad i = 0, 1, \dots, N, \quad h_2 = 4/N,$$

$$\alpha = 10^{-r}, \quad r = 0, 1, \dots, 14.$$

Table 1  
Minimum number of correct digits obtained when solving problem (6.1)–(1.1) with subroutine FIREGU

$\alpha$	Exact data		Perturbed data	
	$N = 16$	$N = 32$	$N = 16$	$N = 32$
1	0.1	0.1	0.1	0.1
$10^{-1}$	0.4	0.4	0.4	0.4
$10^{-2}$	0.5	0.5	0.4	0.4
$10^{-3}$	0.9	0.8	0.7	0.7
$10^{-4}$	1.1	1.1	0.7	0.7
$10^{-5}$	1.1	1.1	0.1 *	-0.2 *
$10^{-6}$	1.6	1.7		
$10^{-7}$	1.2	1.5		
$10^{-8}$	1.3	1.7		
$10^{-9}$	1.1	1.7		
$10^{-10}$	1.0	1.6		
$10^{-11}$	1.0	1.5		
$10^{-12}$	0.7 *	1.3		
$10^{-13}$	0.7 *	1.0 *		
$10^{-14}$	0.4 *	0.1 *		

\* Numerical solution *not* monotonically decreasing.

Table 2  
 Perturbed values  $\hat{g}(x_i)$  of  $g(x_i)$ , used in the test examples

N = 16				N = 32			
$x_i$	$g(x_i)$	$\hat{g}(x_i)$	error (%)	$x_i$	$g(x_i)$	$\hat{g}(x_i)$	error (%)
1.0000	0.510826	0.500345	-2.1	1.0000	0.510826	0.500345	-2.1
1.2667	0.467766	0.476891	2.0	1.1290	0.488975	0.498514	2.0
1.5333	0.431776	0.427548	-1.0	1.2581	0.469034	0.464441	-1.0
1.8000	0.401186	0.409976	2.2	1.3871	0.450752	0.460627	2.2
2.0667	0.374826	0.365242	-2.6	1.5161	0.433920	0.422825	-2.6
2.3333	0.351849	0.352851	0.3	1.6452	0.418367	0.419558	0.3
2.6000	0.331624	0.333124	0.5	1.7742	0.403946	0.405773	0.5
2.8667	0.313673	0.316543	0.9	1.9032	0.390533	0.394106	0.9
3.1333	0.297623	0.301847	1.4	2.0323	0.378022	0.383387	1.4
3.4000	0.283180	0.283277	0.0	2.1613	0.366322	0.366448	0.0
3.6667	0.270109	0.278030	2.9	2.2903	0.355354	0.365775	2.9
3.9333	0.258219	0.263798	2.2	2.4194	0.345050	0.352504	2.2
4.2000	0.247355	0.241919	-2.2	2.5484	0.335348	0.327978	-2.2
4.4667	0.237387	0.239189	0.8	2.6774	0.326197	0.328672	0.8
4.7333	0.228207	0.232738	2.0	2.8065	0.317549	0.323854	2.0
5.0000	0.219722	0.217096	-1.2	2.9355	0.309362	0.305665	-1.2
				3.0645	0.301600	0.305834	1.4
				3.1935	0.294230	0.293497	-0.2
				3.3226	0.287222	0.284772	-0.9
				3.4516	0.280549	0.283210	0.9
				3.5806	0.274188	0.273713	-0.2
				3.7097	0.268116	0.272964	1.8
				3.8387	0.262313	0.269326	2.7
				3.9677	0.256763	0.258344	0.6
				4.0968	0.251448	0.252259	0.3
				4.2258	0.246354	0.240569	-2.3
				4.3548	0.241466	0.237938	-1.5
				4.4839	0.236772	0.236306	-0.2
				4.6129	0.232261	0.228952	-1.4
				4.7419	0.227923	0.228027	0.0
				4.8710	0.223746	0.225888	1.0
				5.0000	0.219722	0.217514	-1.0

For the linear functional  $L$  we chose  $Lf=f$  (zero-order regularization). The initial vector  $\hat{f}$  was taken to be  $\theta$ . In table 1 we give for each test combination of  $\alpha$  and  $N$  the minimum number of correct digits obtained for  $f$  in the mid-points  $\bar{y}_i = \frac{1}{2}(y_{i-1} + y_i)$ ,  $i = 1, 2, \dots, N$ . Since the exact solution is monotonic decreasing, we have marked those cases by an asterisk (\*) for which the numerical solution was *not* monotonically decreasing.

As a second test we have run the same problem with *perturbed* data  $g_i$ , obtained by multiplying  $g(x_i)$ ,  $i = 1, 2, \dots, N$ , by the factor  $1 + 0.03(2\rho - 1)$

where  $\rho$  is a random number in the interval (0,1] generated by the FORTRAN random number generator. Consequently, the maximum perturbation in  $g$  is 3%. In order to facilitate reproduction of our tests, we give in table 2 the perturbed values  $\hat{g}(x_i)$  of  $g(x_i)$  used in our computations, together with the percentages of the perturbation. The results of the second test are given in the part of table 1 with heading "Perturbed data". For  $\alpha < 10^{-5}$  the numerical values of  $f$  obtained were wildly oscillating and completely worthless.

In the case of exact data, the best results were obtained for values of  $\alpha$  which lie in the range

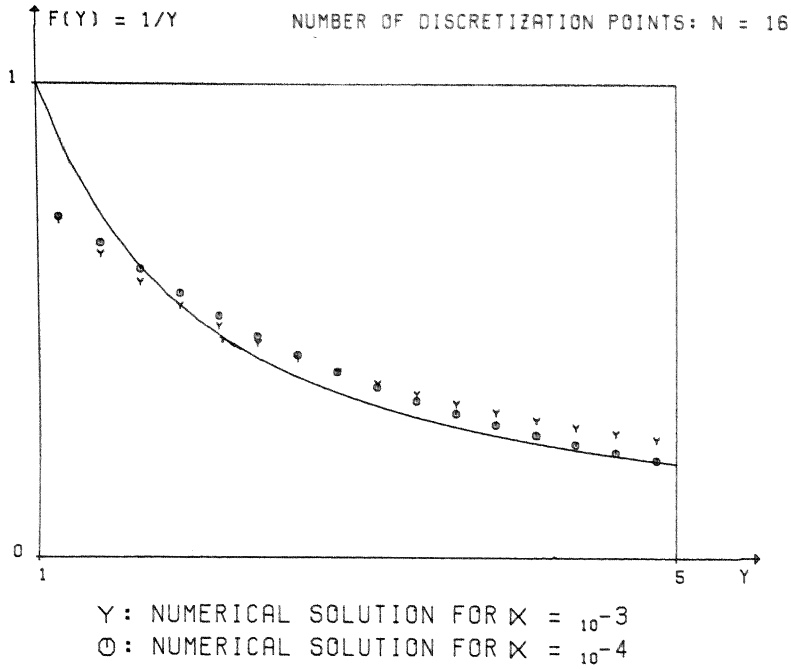


Fig. 1. Numerical solutions  $f_\alpha$  for the cases  $\alpha = 10^{-3}$  and  $10^{-4}$ ,  $N = 16$ .

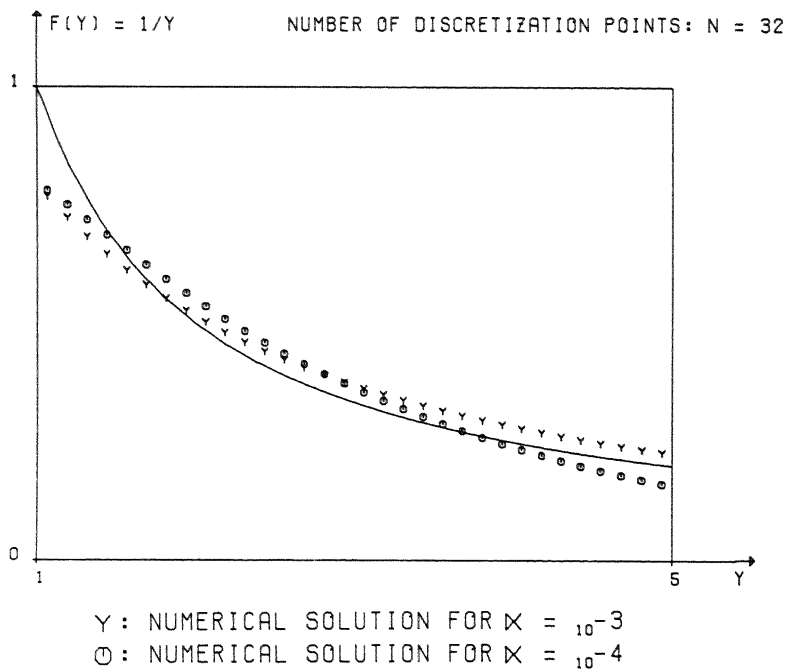


Fig. 2. Numerical solutions  $f_\alpha$  for the cases  $\alpha = 10^{-3}$  and  $10^{-4}$ ,  $N = 32$ .

$10^{-11} < \alpha < 10^{-4}$ . Doubling the number  $N$  of discretization points has some effect only for very small values of  $\alpha$  ( $< 10^{-8}$ , say).

In the case of inexact data, the best results were obtained for  $\alpha = 10^{-3}$  and  $\alpha = 10^{-4}$ . A maximal error of 3% corresponds, roughly, to  $\epsilon = 0.03$  in (2.1). The values of  $\alpha$  for which the best results were obtained agree reasonably well with the theoretical choice  $\alpha = \mathcal{O}(\epsilon^2)$  expressed in (2.2).

In figs. 1 and 2 we present graphs of the numerical solutions  $f_\alpha$  obtained in the cases  $\alpha = 10^{-3}$ ,  $10^{-4}$ ,  $N = 16, 32$ , with inexact data. The drawn line is the exact solution.

The line printer output of the tests shown in figs. 1 and 2 is given below.

The subroutine F1REGU has also been used recently to solve a problem arising in elastic electron-atom scattering [8,12]. Some experiments with a (ALGOL 60) predecessor of F1REGU have been reported in ref. [5].

## References

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## TEST RUN OUTPUT

TEST OF FREGU  
 ORDER OF REGULARIZATION= 0  
 NUMBER OF POINTS N=16 ALFA= .00010000  
 RESIDUES RES(1),...,RES(6)=  
 .1763E+01 .1416E+00 .1100E-01 .2256E-01 .1611E-04 .1103E-01

Y	F(Y) EXACT	F(Y) COMPUTED	NUMBER OF CORRECT DIGITS	ERROR PERCENTAGE
1.125000	.888889	.719862	.7	19.0
1.375000	.727273	.666015	1.1	8.4
1.625000	.615385	.611811	2.2	.6
1.875000	.533333	.560268	1.3	-5.1
2.125000	.470588	.512573	1.0	-8.9
2.375000	.421053	.469044	.9	-11.4
2.625000	.380952	.429594	.9	-12.8
2.875000	.347826	.393959	.9	-13.3
3.125000	.320000	.361803	.9	-13.1
3.375000	.296296	.332782	.9	-12.3
3.625000	.275862	.306564	1.0	-11.1
3.875000	.258065	.282844	1.0	-9.6
4.125000	.242424	.261347	1.1	-7.8
4.375000	.228571	.241827	1.2	-5.8
4.625000	.216216	.224069	1.4	-3.6
4.875000	.205128	.207880	1.9	-1.3

MINIMUM NUMBER OF CORRECT DIGITS: .7

TEST OF FREGU  
 ORDER OF REGULARIZATION= 0  
 NUMBER OF POINTS N=16 ALFA= .00100000  
 RESIDUES RES(1),...,RES(6)=  
 .1751E+01 .1367E+00 .1952E-01 .2297E-01 .3586E-03 .1283E-01

Y	F(Y) EXACT	F(Y) COMPUTED	NUMBER OF CORRECT DIGITS	ERROR PERCENTAGE
1.125000	.888889	.712591	.7	19.8
1.375000	.727273	.641722	.9	11.8
1.625000	.615385	.582561	1.3	5.3
1.875000	.533333	.532537	2.8	.1
2.125000	.470588	.489759	1.4	-4.1
2.375000	.421053	.452814	1.1	-7.5
2.625000	.380952	.420627	1.0	-10.4
2.875000	.347826	.392367	.9	-12.8
3.125000	.320000	.367380	.8	-14.8
3.375000	.296296	.345148	.8	-16.5
3.625000	.275862	.325257	.7	-17.9
3.875000	.258065	.307366	.7	-19.1
4.125000	.242424	.291201	.7	-20.1
4.375000	.228571	.276530	.7	-21.0
4.625000	.216216	.263164	.7	-21.7
4.875000	.205128	.250941	.7	-22.3

MINIMUM NUMBER OF CORRECT DIGITS: .7



## TEST OF F1REGU

ORDER OF REGULARIZATION= 0

NUMBER OF POINTS N=32 ALFA= .00010000

RESIDUES RES(1),...,RES(6)=

.2520E+01 .1196E+00 .4719E-02 .3017E-01 .3131E-03 .1149E-01

Y	F(Y) EXACT	F(Y) COMPUTED	NUMBER OF CORRECT DIGITS	ERROR PERCENTAGE
1.062500	.941176	.781930	.8	16.9
1.187500	.842105	.751169	1.0	10.8
1.312500	.761905	.719359	1.3	5.6
1.437500	.695652	.687305	1.9	1.2
1.562500	.640000	.655555	1.6	-2.4
1.687500	.592593	.624474	1.3	-5.4
1.812500	.551724	.594304	1.1	-7.7
1.937500	.516129	.565195	1.0	-9.5
2.062500	.484848	.537235	1.0	-10.8
2.187500	.457143	.510467	.9	-11.7
2.312500	.432432	.484903	.9	-12.1
2.437500	.410256	.460534	.9	-12.3
2.562500	.390244	.437333	.9	-12.1
2.687500	.372093	.415267	.9	-11.6
2.812500	.355556	.394294	1.0	-10.9
2.937500	.340426	.374369	1.0	-10.0
3.062500	.326531	.355443	1.1	-8.9
3.187500	.313725	.337470	1.1	-7.6
3.312500	.301887	.320402	1.2	-6.1
3.437500	.290909	.304191	1.3	-4.6
3.562500	.280702	.288792	1.5	-2.9
3.687500	.271186	.274162	2.0	-1.1
3.812500	.262295	.260259	2.1	.8
3.937500	.253968	.247042	1.6	2.7
4.062500	.246154	.234474	1.3	4.7
4.187500	.238806	.222519	1.2	6.8
4.312500	.231884	.211143	1.0	8.9
4.437500	.225352	.200314	1.0	11.1
4.562500	.219178	.190001	.9	13.3
4.687500	.213333	.180177	.8	15.5
4.812500	.207792	.170815	.7	17.8
4.937500	.202532	.161889	.7	20.1

MINIMUM NUMBER OF CORRECT DIGITS: .7

## TEST OF F1REGU

ORDER OF REGULARIZATION= 0

NUMBER OF POINTS N=32 ALFA= .001000000

RESIDUES RES(1),...,RES(6)=

.2486E+01 .1138E+00 .9113E-02 .3137E-01 .2840E-04 .1277E-01

Y	F(Y) EXACT	F(Y) COMPUTED	NUMBER OF CORRECT DIGITS	ERROR PERCENTAGE
1.062500	.941176	.768431	.7	18.4
1.187500	.842105	.723721	.9	14.1
1.312500	.761905	.683226	1.0	10.3
1.437500	.695652	.646404	1.2	7.1
1.562500	.640000	.612803	1.4	4.2
1.687500	.592593	.582039	1.7	1.8
1.812500	.551724	.553787	2.4	-.4
1.937500	.516129	.527766	1.6	-2.3
2.062500	.484848	.503736	1.4	-3.9
2.187500	.457143	.481492	1.3	-5.3
2.312500	.432432	.460850	1.2	-6.6
2.437500	.410256	.441655	1.1	-7.7
2.562500	.390244	.423769	1.1	-8.6
2.687500	.372093	.407068	1.0	-9.4
2.812500	.355556	.391447	1.0	-10.1
2.937500	.340426	.376811	1.0	-10.7
3.062500	.326531	.363074	1.0	-11.2
3.187500	.313725	.350161	.9	-11.6
3.312500	.301887	.338005	.9	-12.0
3.437500	.290909	.326545	.9	-12.2
3.562500	.280702	.315727	.9	-12.5
3.687500	.271186	.305501	.9	-12.7
3.812500	.262295	.295824	.9	-12.8
3.937500	.253968	.286655	.9	-12.9
4.062500	.246154	.277957	.9	-12.9
4.187500	.238806	.269698	.9	-12.9
4.312500	.231884	.261847	.9	-12.9
4.437500	.225352	.254377	.9	-12.9
4.562500	.219178	.247262	.9	-12.8
4.687500	.213333	.240480	.9	-12.7
4.812500	.207792	.234008	.9	-12.6
4.937500	.202532	.227828	.9	-12.5

MINIMUM NUMBER OF CORRECT DIGITS: .7