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Numerical treatment of analytic continuation with multiple-precision arithmetic

Hiroshi FUJIWARA, Hitoshi IMAI, Toshiki TAKEUCHI and Yuusuke ISO

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Abstract. The aim of this paper is to show numerical treatment of analytic continuation by high-accurate discretization with multiple-precision arithmetic. We deal with the Cauchy problem of the Laplace equation and an integral equation of the first kind with an analytic kernel. We propose high-accurate discretization based on the spectral method, and show some numerical examples with our proposed multiple-precision arithmetic.

Key words: analytic continuation, ill-posed problem, numerical instability, spectral discretization, multiple-precision arithmetic.

1. Introduction

We consider possibility of numerical treatments of analyticity of functions on digital computers. Analyticity of functions is dependent on the concept of the limit or the infinite, while numerical computations are processed with finite resources. Hence numerical treatment of analyticity has been considered almost impossible because of existence of the rounding errors. Our proposed multiple-precision arithmetic makes them arbitrarily small, and it gives us a clue to realize analytic continuation on digital computers.

We deal with two kinds of analytic continuation from the view point of inverse problems [9]; the one is an initial value problem of the Laplace equation, which is a model of the electrical impedance tomography, and the other is the Fredholm integral equation of the first kind with an analytic kernel, which comes from a model of the X-ray computed tomography. These problems are derived from non-destructive tests in various fields, e.g., engineering, geophysics, and medical science, and they are computed with some regularization methods, which avoid direct numerical treatment of analyticity. On the contrary, with a powerful use of the multiple-precision arithmetic, we dare to approach the problems without any regularization.

The initial value problem of the Laplace equation and an integral equa-

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tion of the first kind with an analytic kernel are typical ill-posed problems in the sense of Hadamard. The ill-posedness is opposite concept to the well-posedness, which means stability of solutions to functional equations against perturbations in given data. Restricting ourselves to linear problems, we can construct their numerically stable schemes and thus reliable numerical solutions, if they are well-posed in the sense of Hadamard. The ill-posed problems are too sensitive to any error entering the problems for us to construct stable numerical schemes. In mathematical analysis, we adopt suitable norms to stabilize the problems: regularization is one of such conventional ways to stabilize ill-posed problems, and numerical treatments of the regularization methods enable us to construct stable numerical schemes. The regularization method, however, contains a parameter, and the schemes have both a discretization parameter and a regularization one. Hence, we note that the choice and the balance of the parameters give another serious difficulty in computations. We focus, in the present research, on the case that we do not admit any errors in data, and we will discretize the problems directly without any regularization. Even under the assumptions, we cannot deal with them with the standard double precision arithmetic, but we can carry them out with our proposed multiple-precision arithmetic.

We will give a brief introduction of our proposed multiple-precision arithmetic and show some numerical examples in the following sections. We discuss, in section 3, the finite difference approach with the multiple-precision arithmetic to an initial value problem of the Laplace equation. We see advantage and difficulty in applications of the multiple-precision arithmetic through examples of 100 digits and 120 digits cases. In sections 4 and 5, we deal with the Fredholm integral equation of the first kind and propose a high-accurate numerical treatment with the spectral collocation method and the multiple-precision arithmetic. We can see the property of analytic continuation through numerical computations, although we do not give a proof here.

2. Multiple-Precision Arithmetic

The multiple-precision environment “exflib” (extended precision floating-point arithmetic library) has been designed and implemented by the first author [4].

In standard numerical computations, the floating-point arithmetic is used to approximate real numbers and their calculations. The double precision arithmetic defined in IEEE754 [7] is commonly used in programming languages and a double precision number has 53 bits precision in binary, which is almost 15 decimal digits accuracy. Thus we can not avoid errors between an exact value and a floating-point number in both representation and arithmetic, which are called the rounding errors. And growth of the rounding errors is serious in the numerical computation of inverse and ill-posed problems.

To reduce the rounding errors, we have proposed the use of the multiple-precision arithmetic, in which we extend a fractional part of a floating-point number as many as possible in order to approximate a real number with arbitrary accuracy. In the number theory or cryptography, a multiple-precision arithmetic has been used, and we propose effective use of ours in scientific computations. Our target is effective process with one hundred up to several thousands decimal digits accuracy for large scale computations coming from numerical analysis of partial differential equations and integral equations. To this end, one of the authors has designed and implemented a new environment of multiple-precision arithmetic, called "exflib", and the environment enables us to deal with numerical computations of ill-posed problems.

The library "exflib" is optimized in some 64-bit computer architectures. It works in FORTRAN90 and in the programming language C++ with seamless interfaces as built-in types for arithmetic expressions, which lead portable and readable codes. It requires less memory than other multiple-precision libraries, and is aimed for large scale and parallel scientific computations. Since the number of fractional digits is variable in exflib, it has a great advantage that we can make the rounding errors arbitrarily small to attain so-called infinitely accuracy virtually. It can be downloaded via the Internet [2].

3. Numerical treatment of analytic continuation

Let $U(z)$ be a holomorphic function on the upper half plane $\{z \in \mathbb{C}; \mathrm{Re}(z) \geq 0\}$, and it satisfies the Cauchy-Riemann equation $\partial U/\partial \bar{z} = 0$. We consider a problem to determine $U(z)$ when its value along the real axis is given. If we write the function $U(z)$ in the form $U(x, y) = u_1(x, y) + iu_2(x, y)$ for $z = x + iy$, the problem is reduced to the Cauchy problem of

$$\frac{\partial}{\partial x}\begin{pmatrix} u_1(x,\,y) \\ u_2(x,\,y) \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \frac{\partial}{\partial y}\begin{pmatrix} u_1(x,\,y) \\ u_2(x,\,y) \end{pmatrix}$$

with the initial values $u_1(x,\,0)$ and $u_2(x,\,0)$, which are given as $U(x,\,0)$. It is well known that the problem is equivalent to that for a harmonic function

$$\triangle u(x,\,y) = 0, \quad (x,\,y) \in \{x \in \mathbb{R},\, y > 0\}, \tag{3.1a}$$

$$u(x,\,0) = f(x), \quad x \in \mathbb{R}, \tag{3.1b}$$

$$\frac{\partial}{\partial y}u(x,\,0) = g(x), \quad x \in \mathbb{R}, \tag{3.1c}$$

where $f(x)$ and $g(x)$ are given real analytic functions. As Hadamard's example shows[10], the harmonic continuation problem (3.1) is ill-posed in Sobolev space H^s of any order $s \in \mathbb{R}$.

We apply the finite difference method (FDM) to seek a numerical solution to (3.1) for $g(x) = 0$. Let Δx and Δy be mesh sizes along x and y axes respectively, and we obtain a finite difference approximation to (3.1) as follows:

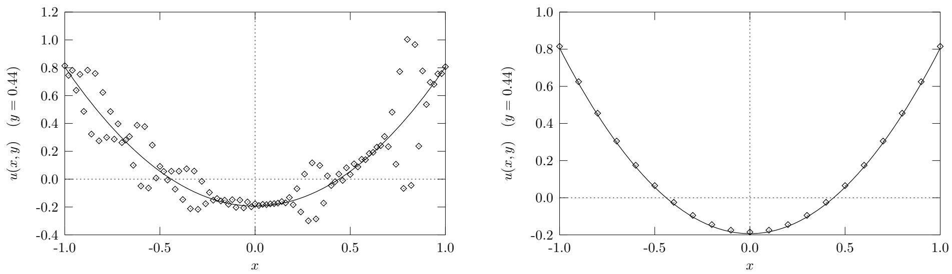
$$\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2} + \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{\Delta y^2} = 0, \quad i \in \mathbb{Z},\, j \geq 1, \tag{3.2a}$$

$$u_{i,0} = f(i\Delta x), \quad i \in \mathbb{Z}, \tag{3.2b}$$

$$u_{i,1} - u_{i,0} = 0. \tag{3.2c}$$

Since the problem (3.1) is ill-posed, the finite difference approximation (3.2) is ill-conditioned and very much sensitive to the rounding errors. Precisely speaking, the finite difference scheme (3.2) is unstable with any Sobolev norm. We should remark that we have a result on convergence of finite difference schemes in the class of analytic functions [6]. For $g(x) = 0$, there exists a unique analytic function $u(x,\,y)$ in some neighborhood of the origin, if $f(x)$ is analytic near $x = 0$, and thus the finite difference solution obtained from (3.2) converges uniformly to the exact one in some neighborhood of the origin as $\Delta x \to 0$ when $\Delta y/\Delta x$ is fixed [6]. The finite difference scheme (3.2) is convergent in the class of analytic functions, although the scheme is unstable with respect to Sobolev norms.

We try to compute the finite difference scheme (3.2) on digital computers for $f(x) = x^2$. The unique solution to (3.1) for $f(x) = x^2$ and $g(x) = 0$ is $u(x,\,y) = x^2 - y^2$, which is a harmonic polynomial. We should remark that



(a) Result in the double precision (b) Result in 100 digits

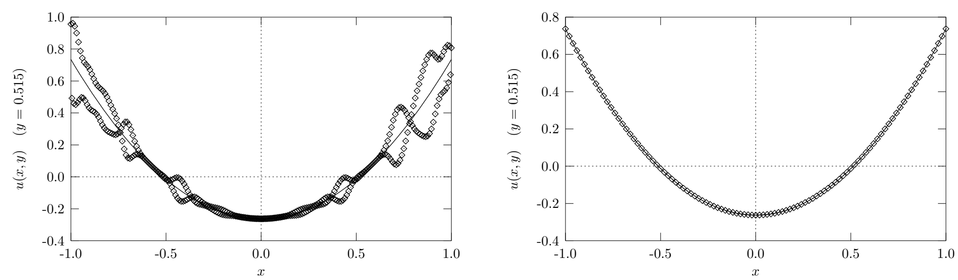
Fig. 1. Numerical solutions to (3.1): $u(x,\, y)$ at $y = 0.44$ for $\Delta x = \Delta y = 0.02$

there occurs no truncation error in the finite difference approximation (3.2) to (3.1) for the case, and the problem of instability is reduced to existence of the rounding errors.

We show some numerical results carried out by the standard double precision arithmetic and the multiple-precision arithmetic. Fig. 1 shows numerical solution at $y = 0.44$ by FDM (3.2) for $\Delta x = \Delta y = 0.02$. Solid curves represent the exact solutions and diamonds ($\diamond$) stand for computed values. Fig. 1(a) computed with the standard double precision shows that the numerical computation clearly fails due to increase of the rounding errors. On the other hand, for the same discretization parameters, we obtain accurate numerical solution shown in Fig. 1(b) in 100 digits with the multiple-precision arithmetic. The figures indicate that the multiple-precision arithmetic enables us to construct numerical solutions which sufficiently approximate the exact solution.

While the multiple-precision arithmetic is quite effective for numerical computations of unstable schemes, it does not essentially remove instability. We compute a numerical solution at $y = 0.515$ by FDM (3.2) for another parameter $\Delta x = \Delta y = 0.005$ in 100 digits, and we show its results in Fig. 2(a). We observe an oscillation due to increase of the rounding errors in Fig. 2(a), and it implies that 100 digits computation is not sufficient for the case. On the other hand, we can obtain a good result in Fig. 2(b) by 120 digits computation.

Analytic continuation is one of the typical ill-posed problems, and we have believed that its direct computation on digital computers should be



(a) Result in 100 digits

(b) Result in 120 digits

Fig. 2. Numerical solutions for $\Delta x = \Delta y = 0.005$, $u(x, y)$ at $y = 0.515$

impossible. The above numerical examples, however, show possibility of numerical analytic continuation, if we use the multiple-precision arithmetic. We remark that necessary number of digits in computation depends on problems, and our multiple-precision arithmetic "exflib" [2] has an advantage that we can easily control accuracy.

4. Integral equations of the first kind and high-accurate discretization

We consider the Fredholm integral equation of the first kind with an analytic kernel on a finite interval I:

$$\int_I k(x, y)u(y)dy = f(x), \quad x \in I. \tag{4.1}$$

Some inverse problems, e.g., the computed tomography and inverse acoustic scattering problems, are often described with integral equations of the first kind with analytic kernels $k(x, y)$, and their numerical analyses are important from the view point of applied inverse problems. Because of analyticity of $k(x, y)$, an integral operator defined by

$$Ku(x) := \int_I k(x, y)u(y)dy. \tag{4.2}$$

is compact on any Sobolev space $H^s(I)$ and does not have a bounded inverse: the problem (4.1) is ill-posed in the sense of Hadamard.

Discretization by the simple collocation method, in which the unknown function u is approximated by a piecewise linear function, does not give us good numerical results because of discretization errors, even if we use the multiple-precision arithmetic to reduce the rounding errors. In order to control discretization errors in exponential order, we propose an application of the spectral method [1, 5], and we remark that discretization of the whole integrand $k(x, y)u(y)$ by the method [8] is more effective than that by the collocation method through numerical examples. Although the method is simple and does not require additional numerical integration, we do not see spectral convergence but polynomial order convergence in numerical experiments in [8]. Hence, to improve convergence order, we will propose another type of application of the spectral method to attain the spectral convergence. Without loss of generality, we take $I = [-1, 1]$ in the following discussion.

Our proposed discretization is based on approximation with the Chebyshev polynomials. Let N be an integer and we approximate the unknown function $u(x)$ by

$$u_N(x) = \sum_{j=0}^{N} u_j T_j(x),$$

where $T_j(x)$ is the Chebyshev polynomial of order j. We choose $\{x_i\}_{i=0}^N \subset I$ as the collocation points and we approximate (4.1) such as

$$\int_{-1}^{1} k(x_i, y) u_N(y) dy = f(x_i), \quad i = 0, 1, \ldots, N.$$

Introducing

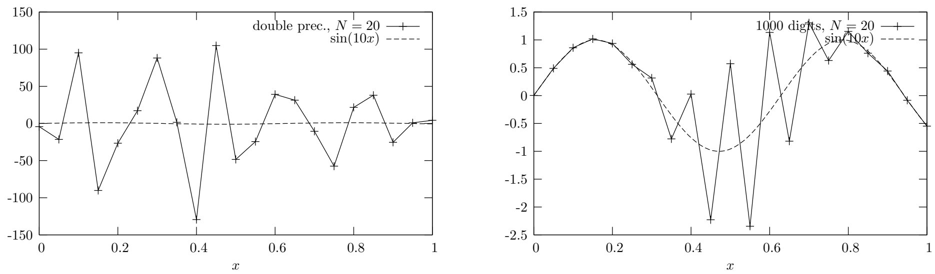
$$K_j(x) := \int_{-1}^{1} k(x, y) T_j(y) dy, \quad k_{ij} := K_j(x_i), \quad K_N := (k_{ij}),$$

we obtain a system of linear equations

$$K_N \big(u_i\big)_{i\downarrow} = \big(f(x_i)\big)_{i\downarrow}.$$

We note that the coefficients $\{k_{ij}\}$ are not obtained exactly in computations, and we need some numerical integration to compute k_{ij}. To this end, we use the following high-accurate numerical integration rule proposed in [3]:

$$\int_{-1}^{1} g(x) dx \approx \frac{\pi}{M} \sum_{j=0}^{M} g(\cos\theta_j) \frac{w_N(\cos\theta_j)}{t_j}, \tag{4.3}$$



(a) Result in the double precision, $N = 20$

(b) Result in 1000 digits, $N = 20$

Fig. 3. Numerical solutions by the simple collocation method

where M is an integer and

$$\theta_j = \frac{\pi}{M} j, \quad w_M(\cos\theta_j) = \frac{2}{\pi}\left(1 + \sum_{\substack{k=2\\ k:\text{even}}}^{M} \frac{2}{1-k^2}\cos\frac{jk\pi}{M}\right).$$

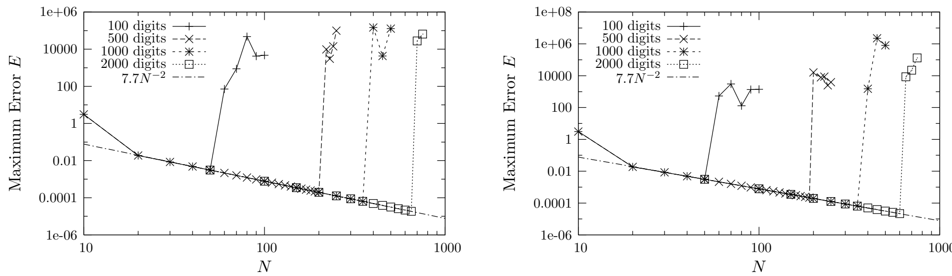
The discretization error in the formula (4.3) decays exponentially with respect to M, if the integrand $g(x)$ is analytic on the interval $[-1, 1]$.

We apply the proposed method to an example

$$\int_0^1 e^{xy} u(y)dy = \frac{xe^x \sin 10 - 10e^x \cos 10 + 10}{x^2 + 100}, \tag{4.4}$$

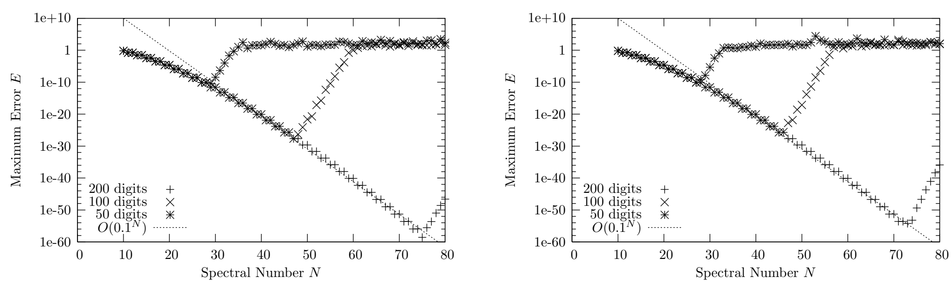
where the exact solution is $u(x) = \sin(10x)$.

Fig. 3 shows numerical solutions by the simple collocation for $N = 20$ in the standard double precision and in 100 digits with the multiple-precision arithmetic respectively. We observe that numerical solutions oscillate and the computations fail. Fig. 4 shows the maximum errors for the previous method proposed in [8]. Fig. 4 (a) is for the case of the Chebyshev-Gauss-Lobatto (CGL) collocation points $\cos(j/N)\pi$, $j = 0, 1, \ldots, N$, and fig. 4 (b) is for that of the equi-spaced points. The horizontal axis stands for the discretization number N, and the vertical one stands for the maximum error $E := \max_{0\le j\le N} |u(x_j) - u_N(x_j)|$, where $\{x_j\}$ is a set of CGL sampling points. We see that the numerical solution converges with polynomial order $O(N^{-2})$.



(a) CGL collocation points (b) Equi-spaced collocation points

Fig. 4. Maximum error E by the previous method in [8]



(a) CGL collocation points (b) Equi-spaced collocation points

Fig. 5. Maximum error E by the proposed method

Fig. 5 shows the maximum error by the present method in which we take $M = 400$ for the numerical integration rule (4.3). We observe the convergence of $O(0.1^N)$ and we note that the spectral accuracy is attained. Hence we conclude that the proposed method is more accurate than the previous one.

5. Numerical analytic continuation for integral equations with analytic kernels

The method shown in the previous section gives spectral convergence with respect to N for both the CGL collocation case and the equi-spaced collocation one. The results are thought to be derived from analyticity and

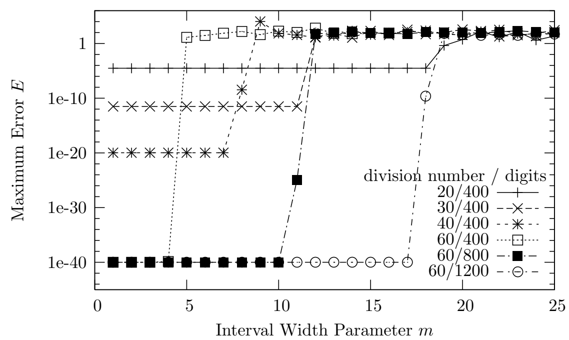


Fig. 6. Numerical error E for local collocation points

we give other numerical examples, in the present section, to ensure the fact.

Since we have the identity theorem for analytic functions, all the information about a function can be derived from its values on sub-interval for an analytic function. We apply the proposed method with the equi-spaced collocation points, but we allocate them only in a sub-interval $J_m = [1/2 - 10^{-m}, 1/2 + 10^{-m}]$. Fig. 6 shows the maximum errors in numerical experiments, where the horizontal axis stands for m. For the case $m = 15$, although the interval J_m is quite small, we see that the numerical solution coincides well with the exact one by 1200 digits computation, and we succeed in reconstruction of an analytic function $u(x)$ from data on a sub-interval.

The numerical results suggest realization of the identity theorem on a digital computer with a combination of the multiple-precision arithmetic and the proposed high-accurate spectral discretization. We recall that our multiple-precision arithmetic has "infinitely" accuracy, since we can make the rounding error arbitrarily small by the change of number of the fractional digits. We should remark that we cannot see the same kind of results by the standard floating-point arithmetic.

6. Concluding Remarks

Analytic continuation related to the Cauchy problem of the Laplace equation and the Fredholm integral equation of the first kind are successfully realized on digital computers by the combination of the multiple-precision arithmetic and the spectral method. The multiple-precision arithmetic enables numerical realization of the Hayakawa's theorem [6] and of the identity theorem for analytic functions through computations, and it gives us a new clue to deal with inverse and ill-posed problems.

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H. Fujiwara
Graduate School of Informatics
Kyoto University
Kyoto 606-8501, Japan
E-mail: fujiwara@acs.i.kyoto-u.ac.jp

H. Imai
The University of Tokushima

T. Takeuchi
The University of Tokushima

Y. Iso
Kyoto University