Publ. RIMS, Kyoto Univ.
41 (2005), 979–988

Complex Function Theory and Numerical Analysis*

By

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What we deal with in computation in physics, for example, is usually a function expressed in terms of a single formula like an algebraic function or an elementary transcendental function, etc. In some cases it involves the symbol of differentiation or that of integration, or it is given implicitly as a solution of some differential equation whose coefficients consist of such functions. In any case such a function is an analytic function handled in the complex function theory. Actually I dare to say that more than 90 percent of practical applications of mathematical analysis deal with analytic functions. Nevertheless, in conventional textbooks on numerical analysis almost all functional algorithms such as interpolation, numerical integration, and numerical differentiation are dealt with in the framework of only the elementary calculus or, in other words, techniques in the theory of real functions. This seems strange to me. We have successfully shown that methods based on the complex function theory are quite efficient in a number of problems of numerical computation, in particular in numerical integration [1]. In what follows, we show other examples in which methods based on the complex function theory are useful and also point out some flaws of the conventional methods.

§1. Significance of the Use of Complex Function Theory

Differentiation, integration and solution of differential equation, etc., are usually an operation on functions of continuous variables. When we carry out actual computation for such operations in a computer or other digital equipments we must first approximately replace the continuous operand with finite and discrete numerical parameters. Then we carry out computation for these

Communicated by H. Okamoto. Received June 9, 2005. Revised August 23, 2005.

*The present paper is a faithful English translation by Masatake Mori with assistance by Hisashi Okamoto of the original Japanese paper published in 1975, in RIMS Kôkyûroku (workshop proceedings) No.253, pp.24–37.

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numerical values and get information about the consequence of differentiation, integration, etc. from the result of computation (which again consists of finite number of parameters). For such finite number of parameters we use, in many cases, function values (sample values) at discrete values of the independent variable (sample points). Sometimes we also use coefficients of an expansion in terms of some suitable set of functions (power series or the Fourier series, for example). However, in any case, in order to express a function in sufficiently high precision with a relatively small number of parameters it is required that the function is moderately smooth (or natural). Although in many books the requirement on the smoothness is not so explicitly mentioned, it is implicitly included in the error representation of the numerical formula. In fact, in many cases the error representation of numerical formulas includes the maximum absolute value of the nth order derivative of the function in question (n is determined depending on the formula), and hence it is implicitly assumed that the function is n-times differentiable and that its n-th order derivative is not very large. However, in practical applications, it is quite rare that, for example, we know that the function is three times differentiable but do not know whether it is four times differentiable or not. In actual applications, on the other hand, it is usually assumed implicitly that the function under consideration is infinite times differentiable, or more strongly, is analytic in a region which includes the real axis. In addition, there are many cases in which the analyticity can actually be proved in some explicitly given region. This is obviously the case if the function is defined explicitly in an analytical form. As another example from the solid state physics, there is a strong reason to believe that the function which describes the current-voltage characteristics of a certain electronic device, a diode for example, is regular in the strip region about the real axis with half width $2\pi kT$ (where k is the Boltzmann constant and T is the absolute temperature). Also, to investigate what kind of analyticity the state function of a material has, or in other words, where and what kind of singularities exist in the complex plane, is an important subject in the field of recent statistical mechanics. As seen from the discussion given above we should recognize that it is by far more realistic to study in what region the function is regular rather than to establish the n times differentiability.

If we base our argument on the analyticity of the function in this way, the complex function theory, in particular Cauchy's integral formula, will play a fundamental role as a matter of course. This will be exemplified in what follows.

§2. On Interpolation

We consider here interpolation. Interpolation is a method to express an unknown function $f(x)$ approximately in terms of its sample values

$$y_1 = f(x_1),\ y_2 = f(x_2), \ldots\ldots,\ y_n = f(x_n). \tag{1}$$

Interpolation formulas in common use are always *linear interpolation*, i.e., interpolation formulas $\bar{f}(x)$ expressed in the form $\bar{f} = \sum c_i(x)f(x_i)$. The most commonly used interpolation is the one based on polynomials (the Lagrange interpolation) in which we assume that $\bar{f}(x)$ is a polynomial of degree $n-1$ and determine the coefficients in such a way that it satisfies (1). Although the sample points x_1, x_2, …, x_n can be chosen arbitrarily, they are usually taken equidistantly. Several other interpolation formulas such as Newton's and Stirling's formulas use a difference table. But the distinction among these formulas lies only in computational algorithm and they are all the same as the Lagrange interpolation from the algebraic point of view (i.e., as long as the round-off error is neglected).

There are two strategies to reduce the error of Lagrange interpolation: (1) to decrease the interval of sample points h, (2) to increase the number of sample points n. However, while decreasing h is always effective for reducing the error, increasing n with fixed h will usually lead to a larger error if n exceeds a certain limit. The resulting $\bar{f}(x)$, which quite often waves up and down violently, becomes a function quite different from the original $f(x)$. This means that the Lagrange interpolation is not suitable for representing a function globally in a single form.

There is another method in which the Lagrange interpolation is used locally in such a way that one uses a Lagrange interpolation formula based on $n = 2\ell$ (even) points only on the central interval, and every time one moves to the adjacent interval one switches the formula by shifting simultaneously all the sample points to be used. Although this method works well as long as n is not very large, one unavoidably encounters a discontinuity, due to the switchover of the local formulas, when x goes across sample points. While $\bar{f}(x)$ itself is of course continuous there, its derivative $\bar{f}'(x)$ is discontinuous. Although the so called spline interpolation is known in which such a discontinuity of $\bar{f}'(x)$ does not appear, one encounters another discontinuity at higher order derivatives and hence it also seems to be a cheap trick.

There is a global interpolation formula in which such a discontinuity does not appear. It is a formula of convolution type, i.e.,

$$\bar{f}(x) = \sum_n \phi(x - nh) f(nh), \tag{2}$$

where $\phi(x)$ satisfies

$$\phi(0) = 1, \quad \phi(nh) = 0 \quad (n = \text{integer} \neq 0). \tag{3}$$

If $\phi(x)$ is analytic on the real axis, then $\bar{f}(x)$ is analytic there, and if $\phi(x)$ is n-times differentiable then $\bar{f}(x)$ is also n-times differentiable. In addition, the Lagrange interpolation formula in which the base interpolation formulas are joined as explained above can be expressed in the form of (2). In that case $\phi(x)$ is not a single function but a mixed function in which a number of polynomials are joined at the points of integer multiples of h (Fig. 1). We call

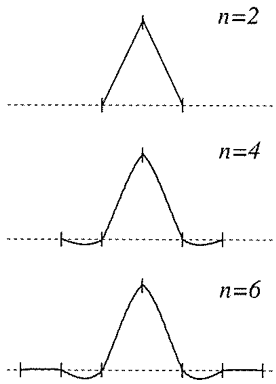

Figure 1.

the function $\phi(x)$, including such a mixed function as above, an *interpolator*.

A typical analytic interpolator is given by

$$\phi(x) = \frac{h}{\pi x} \sin \frac{\pi x}{h}. \tag{4}$$

This gives Shannon's interpolation formula which plays a fundamental role in information theory. This is nothing but a limit of the Lagrange interpolation formula as $n \to \infty$ and, in addition, it has a significant characteristic that it is a *self-consistent* interpolation. An interpolation is called self-consistent, if the following condition is satisfied: If the function which results from this interpolation is again interpolated based on a set of new sample points of the same distances as before, it reproduces the same function, i.e.,

$$\bar{f}(x) = \sum \phi(x - nh + \delta)\bar{f}(nh - \delta) \tag{5}$$

for any δ.

Unfortunately, however, Shannon's interpolation formula cannot be used for an algorithm of numerical computation in practical applications because the convergence of the series is extremely slow. Thus our problem comes down to somehow finding, even if we give up self-consistency or some other good features, an interpolation formula of convolution type which is free from discontinuity from the viewpoint of practical purposes and at the same time converges rapidly. In this search, Cauchy's integral theorem is helpful in the error estimation.

§2.1. A new interpolation formula

First we note that both the value and the error of the interpolation formula expressed in terms of the interpolator defined as (4) are given in the form of a complex integral

$$\frac{\sin(\pi x/h)}{2\pi i}\int_C \frac{f(z)dz}{(z-x)\sin(\pi z/h)}, \tag{6}$$

where the singular points of the integrand include, in addition to the singularity of $f(z)$, simple poles $z = x$ and $z = nh$ ($n = 0, \pm 1, \pm 2, \ldots$). We see that if the path C of integration surrounds x in the positive direction the complex integral above coincides with $f(x)$ itself, while if C surrounds all the poles $z = nh$ in the positive direction it coincides $-\bar{f}(x)$. Consequently the integral whose path surrounds all of these poles gives the error

$$\Delta(x) = f(x) - \bar{f}(x).$$

If $f(z)$ does not have a singularity and behaves as

$$f(z) = o\left(e^{\frac{\pi}{h}|\operatorname{Im} z|}\right) \tag{7}$$

as z moves away from the real axis, then the integral (6) tends to 0 as the path of integration moves sufficiently away from the real axis, and hence the error is zero: $\Delta(x) = 0$. The condition (7) is, in fact, equivalent to the condition known in the field of communication theory that $f(x)$ is band-limited. This may be thought of as a condition on the smoothness of $f(x)$.

Now in order to accelerate the convergence of the interpolation formula we consider

$$\phi(x) = \frac{\sin(\pi x/h)}{\pi x/h}\psi(x) \tag{8}$$

which is a modification of (4). Here $\psi(x)$ is an analytic function which satisfies $\psi(0) = 1$ and must approach 0 quickly as $|x|$ becomes large, because it is introduced in order to accelerate the convergence. It turns out that the error of the present interpolation is expressed as

$$\Delta(x) = \frac{\sin(\pi x/h)}{2\pi i} \int_C \frac{\psi(x-z)f(z)dz}{(z-x)\sin(\pi z/h)}. \tag{9}$$

Example 1.

$$\psi(x) = e^{-ax^2/2h^2}$$

In this case $\psi(x-z)$ increases very quickly if z moves parallel to the imaginary axis and hence we cannot deform the path of integration (9) infinitely far away from the real axis. However, since $\psi(x-z)/\sin\frac{\pi z}{h}$ has saddle points at $z = x \pm i\frac{h\pi}{a}$ we can, provided that $f(x)$ does not vary too rapidly, deform the path of integration in such a way that it passes somewhere near these saddle points, and the error $\Delta(x)$ turns out to be of the order of $e^{-\pi^2/2a}|f(x - i\frac{h\pi}{a})|$. Therefore, if we choose $a = 1/4$, for example, we have $e^{-\pi^2/2a} \approx e^{-20} \approx 10^{-8.7}$ and obtain a result with sufficient accuracy for single precision computation.

In this case, in order to take the terms of interpolation up to the term satisfying $e^{-a(x-nh)^2/2h^2} \approx e^{-n^2a/2} \approx e^{-20}$, we have $n = \pm 13$. Of course this holds under the assumption that $f(z)$ is a slowly varying function and does not increase so quickly as z moves parallel to the imaginary axis. If this assumption does not hold, we need to choose a much smaller value for a and then the number of terms becomes much larger.

Example 2.

$$\psi(x) = \cos^m(\alpha\pi x/h)$$

This $\psi(x)$ is a periodic function of x and does not tend to 0 as $x \to \infty$. However, since it becomes very small in a neighborhood of the point satisfying $\alpha x/h$ =half integer, we get an interpolation formula with a very small error if we truncate the series at this point.

A characteristic of this $\psi(x)$ is that the interpolation based on this function is self-consistent if $f(z)$ is a sufficiently mild function (band-limited to $\frac{1-k}{2h}$) with $0 < m\alpha < k < 1$.

§3. On the Power Series Expansion

We consider here another important method to represent a function in terms of discrete parameters. It is a series expansion, in particular, the power series expansion. While the power series expansion has a remarkable merit that for many important functions the series has simple and explicitly known coefficients, it has a weak point in that the region of convergence is confined to the inside of a circle in the complex plane and it does not converge outside the circle even if the function itself varies there in a completely smooth manner. A strategy to remedy this weak point is to prepare several power series and to cover the required region with their circles of convergence. This method in which new power series are successively generated by shifting the origin is nothing but the so called *analytic continuation*. However, the analytic continuation has been devised for the sake of theoretical treatment of complex functions, and one usually encounters a difficulty if one tries to employ it as an actual numerical algorithm. The difficulty is as follows. If one requires the new series up to the nth term, one needs to compute by far larger number of terms than n in the old series, and if one wants to employ such a procedure for several steps the number of terms required in the earlier steps becomes tremendously large and, in addition, one usually cannot know the number of necessary terms in advance. Moreover, a serious loss of significant digits is also anticipated.

Now we propose here a new method which is a generalization of the idea of the analytic continuation. We consider

$$f(x) = \sum a_n x^n \tag{10}$$

and write x as a function in a more general form

$$x = \phi(u) = \sum b_n u^n. \tag{11}$$

If we apply the variable transformation (11) to (10) we have

$$f(x) = f(\phi(u)) = g(u) = \sum c_n u^n. \tag{12}$$

Although there is an algorithm by which $\{c_n\}$ is computed from $\{a_n\}$ and $\{b_n\}$, it gives rise to the same problem as is encountered in the shift of the origin in analytic continuation. However, if we confine ourselves to the case where

$$b_0 = 0 \quad \text{i.e.} \quad \phi(0) = 0, \tag{13}$$

which means that the series of $\phi(u)$ starts with the term u^1, then c_n can be expressed in a finite form consisting only of a_0, a_1, $\ldots$, a_n, b_1, b_2, $\ldots$, b_n. It is equivalent to truncating each of the series (10) and (11) at the nth term, so that we can easily write down the procedure as an operation on polynomials.

The region of convergence of the power series expansion of $g(u)$ derived in this way is also a disk in the u plane. If we map this disk into the x plane the image will become a region which is of course different from the circle of convergence of the series of $f(x)$ and, in many cases, it will be possible for the new series to converge in a region in which the old series does not. By a suitable choice of $\phi(u)$ we can make the series of $g(u)$ converge in a very large region of x. Although the region of convergence will assume a variety of shapes, we see that in general $f(x)$ should not have a singularity inside this region. Consequently it is desirable to look for a mapping function $\phi(u)$ which leads to a region of convergence whose shape is like an ameba that expands its territory keeping itself away from the singularities.

Example.

$$\phi_1(u) = \frac{2u}{1+u}, \quad \phi_2(u) = \frac{4u}{(1+u)^2}, \quad \phi_3(u) = \frac{8u(1+u^2)}{(1+u)^4}$$

Each of these mapping functions arises from

$$1 - x = \left(\frac{1-u}{1+u}\right)^k \quad k = 1, 2, 4. \tag{14}$$

Every function satisfies $\phi(1) = 1$, i.e., not only 0 but also 1 is fixed by the transformations. In addition $x = \infty$ corresponds to $u = -1$.

Suppose that $f(x)$ has singular points (or branch points) only at $x = 1$ and ∞. Then $g(u)$ has singularities at 1 and -1 and hence the radius of convergence is 1. Conversely, if we transfer back the situation to the x plane we see that, with ϕ_1 the series converges in the left half plane bounded by $\mathrm{Re}\, x = 1$ which is a line parallel to the imaginary axis; with ϕ_2 it converges in the entire plane cut along the half real axis from $x = 1$ up to $+\infty$; and with ϕ_3 it converges in the doubly sheeted entire plane until we reach another cut from $x = 1$ to $-\infty$ (in the negative direction) on the second sheet which we find by crossing the above mentioned cut.

If we take k larger than four, a singularity appears inside the unit circle in the u plane and hence the radius of convergence becomes less than 1, so that the advantage of transformation will become smaller. There is a transformation that is free from such a drawback. It corresponds to the Landen transformation of an elliptic function. The optimal transformation obtained as a limit of such a function is given by the elliptic modular function

$$x = \phi_4(u) \equiv \frac{16u(1+u^2+u^6+u^{12}+\cdots)^4}{(1+2u+2u^4+2u^9+\cdots)^4}. \tag{15}$$

The correspondence under this mapping is

$$\phi(0) = 0, \quad \phi(1) = 1, \quad \phi(-1) = \infty, \quad \phi(-e^{-\pi}) = -1, \quad \phi(e^{-\pi}) = 1/2,$$

and it maps the unit disk in the u-plane infinitely many times onto the x plane except 1 and ∞.

§3.1. Variable transformation as analytic continuation

Variable transformations of this kind not only enlarge the region of convergence but also accelerate slowly convergent series. Hence the scope of applications of such transformations is large in that it can be used as a method of summation which enables us to evaluate a nonconvergent series or a method of acceleration on series.

This variable transformation can also be regarded as a kind of analytic continuation. By means of this method we can investigate the behavior of a function defined in terms of a power series expansion, for example a function defined as

$$\zeta(x,s) = \sum_{n=1}^{\infty} x^n/n^s,$$

on the Riemann surface far from the principal sheet. Although it is a restriction that we cannot move the origin $x = 0$ because it always corresponds to $u = 0$, we can freely choose $\phi(u)$ in other respects, and accordingly, in principle, we can enlarge the region of convergence as largely as we like. In contrast to the conventional analytic continuation it is a remarkable characteristic of the present method that it can be carried out in a single step. Although it may be divided into several steps, the same result can be obtained in a single step, so that it is useless to divide it into more than one step as is required in the conventional analytic continuation. However, it should be noted that even when we employ this method the value of $|u|$ will approach the radius of convergence if we try to reach very far in the x plane, so that the convergence of the series deteriorates in this case.

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Translators' notes

- The original paper was read at the RIMS Workshop "Suuchi Kaiseki to Konpyûta" (Numerical Analysis and Computer) held in October 31–November 2, 1974. The translation plan was approved by Professor Takahasi's survived family. Translators acknowledge with gratitude the helpful comments by Professor Masaaki Sugihara and two anonymous referees. However, only translators are to be blamed for any remaining mistranslations.
- The author, Professor Hidetosi Takahasi, was born on January 15th, 1915, and passed away on June 30th, 1985. He was a renowned physicist, but he is also famous in the applied mathematics community for the DE formulas and other inventions in numerical analysis. He is considered to be one of the pioneers of Japanese computer science. A purple ribbon medal was awarded on him in 1975 by the Japanese government. In 1980, he was elected to a person of cultural merits — one of the highest honors in Japan.