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On the numerical evaluation of Cauchy principal value integrals

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Abstract A generalization of the methods of numerical integration rendering them applicable to the numerical evaluation of Cauchy type singular integrals is given. The method used is based on the theory of complex variables, the Cauchy residue theorem and the Plemelj formulae. Possible further generalizations are also mentioned.

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1. Introduction

Cauchy type integrals of the form

$$\Phi(z) = \frac{1}{2\pi i}\int_L \frac{w(\tau)\phi(\tau)}{\tau - z}\,\mathrm{d}\tau, \tag{1}$$

where L is a part $[a,b]$ of the real axis, $w(\tau)$ is a weight function defined on the interval $[a,b]$, $\phi(z)$ is an analytic function without poles in a domain Ω containing the interval L and surrounded by

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a closed contour C and $\Phi(z)$ is a sectionally analytic function in the whole complex plane except L are often encountered in problems of mathematical physics.

When the point z is not a point of the interval L, the Cauchy type integral (1) generally exists in the ordinary sense provided that the function $w(\tau)\phi(\tau)$ does not present strong singularities of the order -1 or smaller at any point τ of the interval L, but only weak singularities at a finite number of points of the interval L. On the contrary, when the point z lies on the interval L (denoted by t in this case), the Cauchy type integral (1) diverges and is usually defined in the sense of the principal value, i.e. as the limiting value

$$\Phi(t) := \lim_{\varepsilon\to 0} \frac{1}{2\pi i} \int_{L-l} \frac{w(\tau)\phi(\tau)}{\tau - t}\,\mathrm{d}\tau, \quad t \in L. \tag{2}$$

In this expression, the integral extends on the interval L except a small part $l = l(\varepsilon)$ of this interval contained in a circle of radius ε with the singular point t as its centre.

A sufficient condition for the existence of the integral (2) is that its density $w(\tau)\phi(\tau)$ be a Hölder-continuous function in the interval L except in the neighbourhoods of its end-points a and b, where it may present weak singularities. It can also be noticed that when the singular point t coincides with one of the end-points a and b of the interval $L = [a,b]$, the integral (2) does not exist.

The properties of functions $\Phi(z)$ defined as Cauchy type integrals in Eq. (1) were completely investigated long ago and they can be found in several books, among which we can mention Muskhelishvili's monograph on singular integral equations [1]. Among these properties, the most important are the well-known Plemelj formulae relating the limiting values $\Phi^{\pm}(t)$ of the function $\Phi(z)$ when the point z tends to a point t of the interval L from the positive or from the negative half-plane, respectively, to the value $w(t)\phi(t)$ of the density of the integral (1) at the point t and the value $\Phi(t)$ of the function $\Phi(z)$ at this point defined in the sense of the principal value. The Plemelj formulae can be written as [1]

$$\Phi^{+}(t) - \Phi^{-}(t) = w(t)\phi(t), \tag{3}$$

$$\Phi^{+}(t) + \Phi^{-}(t) = 2\Phi(t) = \frac{1}{\pi i} \fint_{L} \frac{w(\tau)\phi(\tau)}{\tau - t}\,\mathrm{d}\tau. \tag{4}$$

The second of these formulae may also serve as an alternative definition of the value $\Phi(t)$ of the function $\Phi(z)$ on the points of the interval L, i.e.

$$\Phi(t) := \frac{1}{2}\left[\Phi^{+}(t) + \Phi^{-}(t)\right]. \tag{5}$$

Then the definition (2) of the function $\Phi(t)$ as a principal value integral could result as a property of its alternative definition (5).

For the numerical evaluation of a Cauchy type integral of the form (1) with the point z not lying on the interval L, it is quite possible to use a numerical integration rule (quadrature rule) for regular integrals. If we consider such a rule of the form

$$\int_{L} w(\tau)\phi(\tau)\,\mathrm{d}\tau = \sum_{k=1}^{n} A_k \phi(\tau_k) + E_n\,, \tag{6}$$

where τ_k are the abscissae (the nodes), A_k are the weights and E_n is the error term in this numerical integration rule, the following formulae are valid [2]

$$A_k = \frac{2q_n(\tau_k)}{\sigma_n'(\tau_k)}\,, \tag{7}$$

$$E_n = \frac{1}{\pi i} \oint_{C} \phi(z')\,\frac{q_n(z')}{\sigma_n(z')}\,\mathrm{d}z', \tag{8}$$

where the closed contour C surrounds the interval L and the functions $\sigma_n(z)$ and $q_n(z)$ are defined by

$$\sigma_n(z) := \prod_{k=1}^{n}(z-\tau_k), \tag{9}$$

$$q_n(z) := -\frac{1}{2}\int_L \frac{w(\tau)\sigma_n(\tau)}{\tau - z}\,\mathrm{d}\tau. \tag{10}$$

It must also be noted that for the points t of the integration interval L the function $q_n(z)$ is defined according to Eqs. (2) or (5) and also that, in general, the selection of the abscissae (the nodes) τ_k $(k=1,2,\ldots,n)$ of the quadrature rule (6) may be arbitrary on the interval L with its end-points a and b included in this interval.

For a Cauchy type integral of the form (1) and for a point z lying inside the closed contour C but not on the interval L, obviously, we have to take into account the pole of the integrand at the point $\tau = z$. Then, following Donaldson and Elliott [2], we will have

$$2\pi i\Phi(z) = \int_L \frac{w(\tau)\phi(\tau)}{\tau - z}\,\mathrm{d}\tau = \sum_{k=1}^{n} A_k \frac{\phi(\tau_k)}{\tau_k - z} - 2\phi(z)\frac{q_n(z)}{\sigma_n(z)} + E_n\,, \quad z \notin L, \tag{11}$$

where

$$E_n = \frac{1}{\pi i}\oint_C \frac{\phi(z')}{z'-z}\,\frac{q_n(z')}{\sigma_n(z')}\,\mathrm{d}z'. \tag{12}$$

Now, when the point z of the integral (1) is a point t of the interval L not coinciding with its end-points a and b, a case which is encountered quite frequently, unfortunately, up to now there has not been developed a general method for extending the rules of numerical integration so that they can become applicable to the numerical evaluation of such an integral. Only recently, Hunter [3] and Chawla and Ramakrishnan [4] extended the use of the Gauss–Legendre and the Gauss–Jacobi numerical integration rules, respectively, to the numerical evaluation of Cauchy principal values of integrals.

Here we will extend, in a general way, the methods of numerical integration rendering them applicable to the evaluation of Cauchy principal value integrals. In this extension, we will use a method similar to the method already used in Refs. [3] and [4] for the aforementioned numerical integration rules as well as a new method developed here for the first time and based on the Plemelj formulae (3) and (4).

Finally, we can remark that the correct definition of the principal value of a Cauchy type integral is not that given in Refs. [3] and [4] but that given in Eq. (2).

2. Direct method of evaluation of Cauchy principal value integrals

For the evaluation of a Cauchy principal value integral (1) with the point z coinciding with a point t of the interval $L=[a,b]$ except its end-points a and b and also except the roots τ_k of the function (the polynomial) $\sigma_n(z)$ defined by Eq. (9), following Hunter [3] and Chawla and Ramakrishnan [4], we consider the following contour integral on the closed contour C surrounding the interval L (Fig. 1):

$$I_0 = \frac{1}{2\pi i}\oint_C \frac{\phi(z')}{(z'-t)(z'-z)\sigma_n(z')}\,\mathrm{d}z', \quad t \in L, \tag{13}$$

where the function $\sigma_n(z)$ is the polynomial defined by Eq. (9).

By applying the Cauchy residue theorem to this integral I_0, we find

$$\frac{\phi(z)}{(z-t)\sigma_n(z)} = \sum_{k=1}^{n}\frac{\phi(\tau_k)}{\tau_k - t}\,\frac{1}{(z-\tau_k)\sigma_n'(\tau_k)} + \frac{\phi(t)}{(z-t)\sigma_n(t)} + \frac{1}{2\pi i}\oint_C \frac{\phi(z')}{(z'-t)(z'-z)\sigma_n(z')}\,\mathrm{d}z'. \tag{14}$$

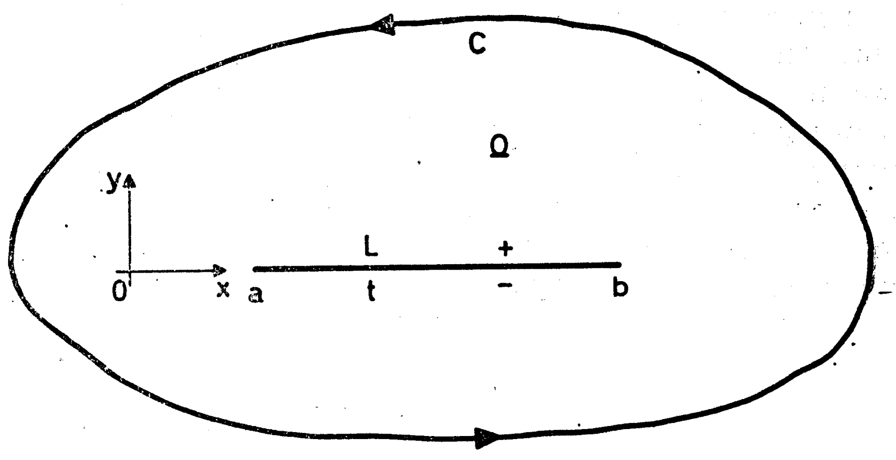

Fig. 1: Geometry of the integration interval L and the contour C

If we replace this expression of the function $\phi(z)$ in the integral (1) for a point t of the interval L, we obtain

$$2\pi i\Phi(t) = \int_L \frac{w(\tau)\phi(\tau)}{\tau - t}\,\mathrm{d}\tau = \sum_{k=1}^{n} A_k \frac{\phi(\tau_k)}{\tau_k - t} - 2\phi(t)\frac{q_n(t)}{\sigma_n(t)} + E_n, \quad t \in L, \quad \sigma_n(t) \neq 0, \tag{15}$$

where

$$E_n = \frac{1}{\pi i}\oint_C \frac{\phi(z')}{z' - t}\frac{q_n(z')}{\sigma_n(z')}\,\mathrm{d}z', \tag{16}$$

i.e. we obtain the same expression as in the case when the point z was not a point t of the interval L when Eq. (11) has been obtained. The only remark that we have to make here is that the value $q_n(t)$ of the function $q_n(z)$ for $z = t$ in Eq. (15) should be calculated in the sense of the principal value.

Equation (15) means that any numerical integration rule of the general form (6) for regular integrals can also be used for the evaluation of Cauchy type principal value integrals without any change in the values of the abscissae τ_k and the weights A_k used provided that one more term, i.e. the term due to the pole of the integrand at the singular point $\tau = t$, is added.

3. Evaluation of Cauchy principal value integrals on the basis of the Plemelj formulae

Under the same assumptions as in the previous section, Section 2, in this section we will calculate a Cauchy principal value integral by using the Plemelj formulae. At first, we apply the two Plemelj formulae (3) and (4) to the function $q_n(z)$ defined by Eq. (10). Then we obtain

$$q_n^+(t) - q_n^-(t) = -\pi i w(t)\sigma_n(t), \tag{17}$$

$$q_n^+(t) + q_n^-(t) = -\int_L \frac{w(\tau)\sigma_n(\tau)}{\tau - t}\,\mathrm{d}\tau. \tag{18}$$

By using Eq. (11), Eqs. (17) and (18) can be used to obtain the limiting values $\Phi^{\pm}(t)$ of the function $\Phi(z)$ of Eq. (1) near the points t of the interval L. Then, taking also into consideration the Plemelj formulae (3) and (4), we find

$$\begin{aligned} 2\pi i\Phi^{\pm}(t) &= \lim_{z\to t^{\pm}} \int_L \frac{w(\tau)\phi(\tau)}{\tau - z}\,\mathrm{d}\tau \\ &= \pm\pi i w(t)\phi(t) + \int_L \frac{w(\tau)\phi(\tau)}{\tau - t}\,\mathrm{d}\tau \\ &= \sum_{k=1}^{n} A_k \frac{\phi(\tau_k)}{\tau_k - t} \pm \pi i w(t)\phi(t) - 2\phi(t)\frac{q_n(t)}{\sigma_n(t)} + E_n. \end{aligned} \tag{19}$$

From this equation and because of Eq. (5), Eq. (15) is directly deduced. At this point, we can remark that the real meaning of Eq. (15) consists in the evaluation of a Cauchy principal value integral $\Phi(t)$ through the use of another principal value integral $q_n(t)$. When we use this numerical integration rule, Eq. (15), it is assumed that we know the function $q_n(t)$ corresponding to the numerical integration rule (6) that we use either in a closed form or in an easy to compute form.

4. The case of coincidence of the point t with an abscissa τ_k

In Sections 2 and 3 we have excluded the case when the singular point t in the interval $L=[a,b]$ coincides with an abscissa τ_k $(k=1,2,\ldots,n)$ of the numerical integration rule (6). Now we consider the case where the point t coincides with an abscissa τ_m $(m=1,2,\ldots,n)$. Of course, the point τ_m should be different from the end-points a and b of the integration interval $L=[a,b]$. In the present case, by applying the Cauchy residue theorem to the integral (13), we find

$$\begin{aligned}\frac{\phi(z)}{(z-t)\sigma_n(z)} &= \sum_{\substack{k=1\\k\neq m}}^{n} \frac{\phi(\tau_k)}{\tau_k-t}\,\frac{1}{(z-\tau_k)\sigma_n'(\tau_k)} + \frac{\phi'(\tau_m)}{(z-\tau_m)\sigma_n'(\tau_m)} \\ &\quad + \frac{\phi(\tau_m)}{(z-\tau_m)\sigma_n'(\tau_m)}\left[\frac{1}{z-\tau_m} - \frac{\sigma_n''(\tau_m)}{2\sigma_n'(\tau_m)}\right] + \frac{1}{2\pi i}\oint_C \frac{\phi(z')}{(z'-t)(z'-z)\sigma_n(z')}\,\mathrm{d}z'. \quad (20)\end{aligned}$$

Then Eq. (15) is modified as

$$\begin{aligned}2\pi i\Phi(\tau_m) = \int_L \frac{w(\tau)\phi(\tau)}{\tau-\tau_m}\,\mathrm{d}\tau &= \sum_{\substack{k=1\\k\neq m}}^{n} A_k\,\frac{\phi(\tau_k)}{\tau_k-\tau_m} + A_m\phi'(\tau_m) \\ &\quad - 2\phi(\tau_m)\,\frac{1}{\sigma_n'(\tau_m)}\left[q_n'(\tau_m) + \frac{1}{4}A_m\sigma_n''(\tau_m)\right] + E_n\,, \quad (21)\end{aligned}$$

where the integral

$$q_n'(\tau_m) = -\frac{1}{2}\int_L \frac{w(\tau)\sigma_n(\tau)}{(\tau-\tau_m)^2}\,\mathrm{d}\tau \quad (22)$$

can be computed in the sense of the principal value since τ_m is a root of the polynomial $\sigma_n(z)$.

In another way of thinking, Eq. (21) can be obtained from Eq. (15) if the singular point t $(t\in L)$ tends to the point τ_m. If we put $t-\tau_m=\delta$, we find that

$$\begin{aligned}&\lim_{\delta\to 0}\left[A_m\,\frac{\phi(\tau_m)}{-\delta} - 2\phi(\tau_m+\delta)\,\frac{q_n(\tau_m+\delta)}{\sigma_n(\tau_m+\delta)}\right] \\ &\quad = A_m\phi'(\tau_m) - 2\phi(\tau_m)\,\frac{1}{\sigma_n'(\tau_m)}\left[q_n'(\tau_m) + \frac{1}{4}A_m\sigma_n''(\tau_m)\right] + E_n\,, \quad (23)\end{aligned}$$

where Eq. (7) giving the weights A_k has also been taken into account.

One third way for obtaining the quadrature rule (21) consists in modifying Eq. (11) for the case when the point z tends to an abscissa τ_m $(m=1,2,\ldots,n)$. In this case, putting $z-\tau_m=\delta$ (with $\operatorname{Im}\delta\neq 0$), we find, after taking into consideration an equation analogous to Eq. (23), that

$$2\pi i\Phi^{\pm}(\tau_m) = \sum_{\substack{k=1\\k\neq m}}^{n} A_k\,\frac{\phi(\tau_k)}{\tau_k-\tau_m} + A_m\phi'(\tau_m) - 2\phi(\tau_m)\,\frac{1}{\sigma_n'(\tau_m)}\left[q_n'^{\pm}(\tau_m) + \frac{1}{4}A_m\sigma_n''(\tau_m)\right] + E_n\,. \quad (24)$$

As regards the function $q_n'(z)$, it results simply by a differentiation of Eq. (10). Then we obtain

$$q_n'(z) = -\frac{1}{2}\int_L \frac{w(\tau)\sigma_n(\tau)}{(\tau-z)^2}\,\mathrm{d}\tau. \quad (25)$$

In general, the function $q'_n(z)$ is not defined on the points t of the interval $L=[a,b]$. Nevertheless, we can define it on these points too by the following equation, which is analogous to Eq. (5)

$$q'_n(t) := \frac{1}{2}\,[q'^{+}_n(t) + q'^{-}_n(t)]. \tag{26}$$

It can be proved [5] that the limiting values $q'^{\pm}_n(t)$ exist if the function $w(t)\sigma_n(t)$ and its first derivative are Hölder-continuous functions in the interval L except in the neighbourhoods of its end-points a and b. When the point z coincides with an abscissa τ_m, the function $q'_n(t)$ exists in the sense of the principal value and Eq. (26) is simply the second Plemelj formula. In this case, by adding Eqs. (24) and taking into account Eqs. (5) and (26), we again obtain the quadrature rule (21).

5. Generalizations

The methods of numerical evaluation of Cauchy principal value integrals presented here may easily be extended to some more complicated cases in an evident way.

At first, when the interval L is an infinite interval, that is one of its end-points a and b or both of them tend to infinity, we have simply to consider the closed contour C in Fig. 1 also tending to infinity. If only the point a tends to $-\infty$, then the contour C will be composed of two branches, one above the interval L and one below it extending from $-\infty$ up to a point $c > b$ of the real axis, which will be the common point of these branches. If only the point b tends to $+\infty$, the contour C will be composed, in an analogous way, of two branches extending from $+\infty$ up to a point $c < a$ of the real axis. Finally, if the point a tends to $-\infty$ and the point b to $+\infty$, the contour C will be composed of two independent branches, one above the real axis and one below it, extending from $-\infty$ to $+\infty$.

We can also consider the case of Cauchy type integrals of the form (1) where the interval L is not a part of the real axis but it is a smooth curvilinear arc in the complex plane. In this case, if we consider the parametric equations of this arc of the general forms

$$x = x(s), \quad y = y(s), \quad \tau = x + iy = x(s) + iy(s) = \tau(s), \tag{27}$$

where the variable s is a real variable and, possibly, the arc length varying from s_1 (corresponding to the end-point a of the arc L) up to s_2 (corresponding to the other end-point b of the arc L), we can transform the Cauchy type integral (1) into the integral

$$\Phi(z) = \frac{1}{2\pi i}\int_{s_1}^{s_2} \frac{w(\tau(s))\,\phi(\tau(s))}{\tau(s) - z}\,\tau'(s)\,\mathrm{d}s, \tag{28}$$

which now extends on the interval $[s_1, s_2]$ of the real axis. If the point z lies on the arc L coinciding with a point $\tau(\sigma)$ of this arc, we will have as principal value of the Cauchy type integral (28) the integral

$$\Phi(z) = \frac{1}{2\pi i}\int_{s_1}^{s_2} \frac{w(\tau(s))\,\phi(\tau(s))}{s - \sigma}\,\frac{s - \sigma}{\tau(s) - \tau(\sigma)}\,\tau'(s)\,\mathrm{d}s, \quad z \in L, \tag{29}$$

where the term $(s-\sigma)/[\tau(s) - \tau(\sigma)]$ tends to the limit $1/\tau'(\sigma)$ as $s \to \sigma$. This limit exists because it was assumed that the arc L is a smooth curvilinear arc.

The case when we have to evaluate a Cauchy principal value integral of the form (1) along a closed smooth curve L of the complex plane is also of particular interest. Of course, this case can be reduced to the case of a smooth curvilinear open arc by considering the closed curve cut at an arbitrary point $a \equiv b$. But a better approach would be to use the methods of numerical evaluation of integrals of periodic functions since the parametric equations of the general form (27) for a closed curve L are periodic functions of the real variable s, where the period is equal to the length of the curve L in the case when the real variable s denotes the arc length along the curve L.

With respect to this point, we have to mention that the trapezoidal quadrature rule was modified by Chawla and Ramakrishnan [6] so as to become applicable to the evaluation of Cauchy principal value integrals for periodic functions. Then it can also be applied to the evaluation of Cauchy principal value integrals along closed curves. A disadvantage of the trapezoidal quadrature rule lies in the fact that the abscissae used should be equidistant along the real axis and they cannot be arbitrarily selected with the aim to obtain the best possible accuracy. It is hoped that the methods of numerical evaluation of Cauchy principal value integrals presented here and based on an arbitrary selection of the abscissae used will be extended to the case of periodic functions. Then the evaluation of such integrals along closed curves will be more easy and accurate.

Moreover, the case of an integral of the form

$$I = \int_L \frac{w(\tau)\phi(\tau)}{\prod_{i=1}^{l}(\tau - z_i)}\,\mathrm{d}\tau, \tag{30}$$

which is a generalization of the Cauchy type integral (1), can be treated in exactly the same way as the case of the integral (1). It is sufficient that all the poles z_i be taken into account. Then the second term of the right-hand side of Eqs. (11) and (15) should be replaced by a sum of the form

$$R = -2\sum_{k=1}^{l} \frac{\phi(z_k)}{\prod_{\substack{i=1\\ i\neq k}}^{l}(z_k - z_i)}\,\frac{q_n(z_k)}{\sigma_n(z_k)}, \tag{31}$$

where all the poles z_k of the integrand, either lying on the interval L or outside it, are taken into account.

Equation (31) is a generalization of the corresponding equation given by Hunter [3] and by Chawla and Ramakrishnan [4] for the cases of the Gauss–Legendre and the Gauss–Jacobi numerical integration rules, respectively.

One last possible extension of the methods of numerical evaluation of Cauchy principal value integrals is to consider the case of other normally divergent integrals of the form

$$I = \fint_L \frac{w(\tau)\phi(\tau)}{(\tau - t)^k}\,\mathrm{d}\tau, \tag{32}$$

where k is a positive integer, either they are defined in the sense of the principal value or not. In the latter case, an appropriate definition should be given to these integrals before trying to evaluate them numerically. Such a definition was given previously for the function $q_n'(t)$ in Eq. (26).

6. On the evaluation of the function $q_n(t)$

The main disadvantage of the methods for the numerical evaluation of Cauchy principal value integrals lies in the necessity that the function $q_n(t)$ be computed being itself a Cauchy principal value integral too. In general, the computation of such a function, defined by Eq. (10), is not an easy task. Most approximate and asymptotic formulae for the evaluation of functions of the form (10) hold true only for values of the variable z tending to infinity and not lying on the interval L.

Fortunately, in most usually used numerical integration rules, the corresponding functions $q_n(t)$ can be expressed in terms of other functions, the properties of which have been already investigated. A table for the expressions of the functions $q_n(z)$ can be found in Ref. [2] for some well-known numerical integration rules. In more detail, the properties of the functions $q_n(z)$ as well as hints for their numerical computation on the interval L when they are Cauchy principal value integrals for the cases of numerical integration rules based on the properties of orthogonal polynomials, i.e. rules of the Gauss, Radau and Lobatto type, can be found in a paper of Theocaris [7] and the dissertation of Ioakimidis [8].

In these references, it is shown that the functions $q_n(t)$ are simple polynomials in the cases of the Gauss–Chebyshev and the Lobatto–Chebyshev quadrature rules (but only on the integration interval $L=[-1,1]$), easily computed functions with a logarithmic term in the cases of the Gauss–Legendre and the Lobatto–Legendre quadrature rules, hypergeometric functions in the case of the Gauss–Jacobi quadrature rule, where they can be computed only after transformations by using the properties of hypergeometric functions, and confluent hypergeometric functions in the cases of the Gauss–Laguerre and the Gauss–Hermite quadrature rules, where they can be computed through the computation of the exponential integral $\mathrm{Ei}(t)$ and the Dawson integral $F(t)$, respectively.

It is hoped that the properties of the functions $q_n(t)$ on the corresponding integration intervals will be investigated with special attention paid to the number and the location of their zeros, which are of particular importance to the numerical solution of singular integral equations with Cauchy type kernels.

7. Some special quadrature rules

In this section, we will apply the previously developed theory of numerical evaluation of Cauchy type principal value integrals to four well-known numerical integration rules (or quadrature rules), namely the Gauss–Legendre rule (or, simply, the Gauss rule), the Lobatto–Legendre rule (or, simply, the Lobatto rule), the Gauss–Chebyshev rule and the Lobatto–Chebyshev rule.

First, we note that Eqs. (15) and (21) for the evaluation of Cauchy type principal value integrals may also be written as

$$\int_L \frac{w(\tau)\phi(\tau)}{\tau-t}\,\mathrm{d}\tau = \sum_{k=1}^{n} A_k \frac{\phi(\tau_k)}{\tau_k-t} - 2\phi(t)K_n(t) + E_n, \quad t\neq\tau_m, \quad m=1,2,\ldots,n, \tag{33}$$

$$\int_L \frac{w(\tau)\phi(\tau)}{\tau-t}\,\mathrm{d}\tau = \sum_{\substack{k=1\\k\neq m}}^{n} A_k \frac{\phi(\tau_k)}{\tau_k-t} + A_m\phi'(t) - 2\phi(t)\Lambda_n(t) + E_n, \quad t=\tau_m, \quad m=1,2,\ldots,n, \tag{34}$$

respectively, where

$$K_n(t) := \frac{q_n(t)}{\sigma_n(t)}, \quad t\neq\tau_m, \quad m=1,2,\ldots,n, \tag{35}$$

$$\Lambda_n(t) := \frac{1}{\sigma_n'(t)}\left[q_n'(t) + \frac{1}{4}A_m\sigma_n''(t)\right], \quad t=\tau_m, \quad m=1,2,\ldots,n. \tag{36}$$

Of course, the singular point t is not permitted to coincide with an end-point a or b of the integration interval $L=[a,b]$ either it is an abscissa of the numerical integration rule used or not.

Now we will determine the functions $K_n(t)$ and $\Lambda_n(t)$ for the previously mentioned four numerical integration rules, which are the most commonly used rules in applied mechanics problems and have as integration interval the interval $[-1,1]$ of the real axis.

7.1. The Gauss–Legendre quadrature rule [9]

This rule has as weight function $w(t)$ the function $w(t)=1$ or, in other words, it has no weight function. The generalization of this well-known rule for regular integrals to the case of Cauchy type principal value integrals was made by Hunter [3] as was already mentioned in Section 1. The functions $\sigma_n(z)$ and $q_n(z)$ for this rule are [2, 3]

$$\sigma_n(z) = P_n(z), \quad q_n(z) = Q_n(z), \tag{37}$$

where $P_n(z)$ and $Q_n(z)$ denote the Legendre polynomial of degree n and the Legendre function of the second kind and order n, respectively.

Then, Eq. (35) gives

$$K_n(t) = \frac{Q_n(t)}{P_n(t)}, \tag{38}$$

a result agreeing with the developments of Hunter [3].

Furthermore, if we take into account the well-known properties of the Legendre polynomials $P_n(z)$ [10–12]

$$(1-z^2)P_n''(z) - 2zP_n'(z) + n(n+1)P_n(z) = 0, \tag{39}$$

$$(z^2-1)P_n'(z) = nzP_n(z) - nP_{n-1}(z), \tag{40}$$

valid also for the Legendre functions of the second kind $Q_n(z)$, we easily find that

$$\frac{P_n''(t)}{P_n'(t)} = \frac{2t}{1-t^2}, \quad \frac{Q_n'(t)}{P_n'(t)} = \frac{Q_{n-1}(t)}{P_{n-1}(t)} + nA_m \frac{t}{2(1-t^2)}, \quad t = \tau_m, \quad m = 1,2,\ldots,n. \tag{41}$$

Hence, we obtain the following expression for the function $\Lambda_n(t)$ defined by Eq. (36) and valid only for the abscissae τ_m inside the integration interval $(-1,1)$:

$$\Lambda_n(t) = \frac{Q_{n-1}(t)}{P_{n-1}(t)} + \frac{n+1}{2} A_m \frac{t}{1-t^2}. \tag{42}$$

This expression of $\Lambda_n(t)$ can be shown to be equivalent to the expression

$$\Lambda_n(t) = \frac{Q_{n+1}(t)}{P_{n+1}(t)} - \frac{n}{2} A_m \frac{t}{1-t^2} \tag{43}$$

obtained in a different way by Hunter [3].

Finally, as regards the evaluation of the Legendre functions $P_n(z)$ and $Q_n(z)$, the following very well-known recurrence relations for the Legendre polynomials $P_n(z)$ and the Legendre functions of the second kind $Q_n(z)$ [10–12] can be successfully used:

$$nP_n(z) = (2n-1)zP_{n-1}(z) - (n-1)P_{n-2}(z), \tag{44}$$

$$nQ_n(z) = (2n-1)zQ_{n-1}(z) - (n-1)Q_{n-2}(z), \tag{45}$$

$$P_0(z) = 1, \quad P_1(z) = z, \quad Q_0(z) = \frac{1}{2}\ln\frac{1+z}{1-z}, \quad z \in (-1,1), \quad Q_1(z) = zQ_0(z) - 1. \tag{46}$$

7.2. The Lobatto–Legendre quadrature rule [9]

This rule has no weight function $w(t)$ exactly as the Gauss–Legendre rule and it contains among the abscissae used the end-points ± 1 of the integration interval $[-1,1]$. The functions $\sigma_n(z)$ and $q_n(z)$ for this rule have the simple forms [8]

$$\sigma_n(z) = P_n(z) - P_{n-2}(z) = \frac{2n-1}{n(n-1)}(z^2-1)P_{n-1}'(z), \tag{47}$$

$$q_n(z) = Q_n(z) - Q_{n-2}(z) = \frac{2n-1}{n(n-1)}(z^2-1)Q_{n-1}'(z), \tag{48}$$

where $P_n(z)$ and $Q_n(z)$ denote again the Legendre polynomial of degree n and the Legendre function of the second kind and order n, respectively.

Then, Eq. (35) gives

$$K_n(t) = \frac{Q_n(t) - Q_{n-2}(t)}{P_n(t) - P_{n-2}(t)} = \frac{Q_{n-1}'(t)}{P_{n-1}'(t)}. \tag{49}$$

Furthermore, by taking into account Eqs. (39, (40), (44) and (45), we can show that

$$\frac{\sigma_n''(t)}{\sigma_n'(t)} = 0, \quad \frac{q_n'(t)}{\sigma_n'(t)} = \frac{Q_{n-1}(t)}{P_{n-1}(t)}, \quad \begin{cases} t = \tau_m, & m = 2, 3, \ldots, n-1, \\ t \neq t_1, t_n, & t_1 = 1, \quad t_n = -1. \end{cases} \tag{50}$$

Then from Eq. (36) we obtain

$$\Lambda_n(t) = \frac{Q_{n-1}(t)}{P_{n-1}(t)}. \tag{51}$$

This equation is valid only for the abscissae τ_m lying inside the integration interval $(-1, 1)$.

7.3. The Gauss–Chebyshev quadrature rule [9]

This rule has as weight function $w(t)$ the function $w(t) = (1-t)^{\pm 1/2}(1+t)^{\pm 1/2}$ and was applied to the case of Cauchy type principal value integrals by Chawla and Ramakrishnan [4]. Nevertheless, these authors did not consider the case when the Cauchy type principal value integral has to be evaluated at a point coinciding with some of the abscissae used. Here we will consider only the case where $w(t) = 1/\sqrt{1-t^2}$. In this case, the functions $\sigma_n(z)$ and $q_n(z)$ have the simple forms [4, 8]

$$\sigma_n(z) = T_n(z), \quad q_n(z) = -\frac{\pi}{2} U_{n-1}(z), \quad z \in (-1, 1), \tag{52}$$

where $T_n(z)$ and $U_n(z)$ denote the Chebyshev polynomials of the first and of the second kind and of degree n, respectively, easily expressible in terms of trigonometric functions [10–12]. It should also be noted that the second of Eqs. (52) is valid only for the points z of the integration interval $(-1, 1)$.

Then Eq. (35) gives

$$K_n(t) = -\frac{\pi U_{n-1}(t)}{2T_n(t)}. \tag{53}$$

This equation is in accordance with the developments of Ref. [4].

Furthermore, by taking into account the properties of the Chebyshev polynomials [10–12]

$$(1-z^2)T_n''(z) = zT_n'(z) - n^2 T_n(z), \tag{54}$$

$$(1-z^2)T_n'(z) = -nzT_n(z) + nT_{n-1}(z), \tag{55}$$

$$(1-z^2)U_{n-1}'(z) = -(n-1)zU_{n-1}(z) + nU_{n-2}(z), \tag{56}$$

from Eq. (36) we can easily find that

$$\Lambda_n(t) = -\frac{\pi U_{n-2}(t)}{2T_{n-1}(t)} + \frac{2n-1}{4} A_m \frac{t}{1-t^2}. \tag{57}$$

Obviously, this equation is valid only for the abscissae τ_m ($m = 1, 2, \ldots, n$) used.

7.4. The Lobatto–Chebyshev quadrature rule [9]

This rule has the same weight function $w(t)$ as the Gauss–Chebyshev rule and it contains among the abscissae used the end-points ± 1 of the integration interval $[-1, 1]$. Here we will consider again only the case where $w(t) = 1/\sqrt{1-t^2}$. The functions $\sigma_n(z)$ and $q_n(z)$ for this rule have the simple forms [8]

$$\sigma_n(z) = 2(z^2-1)U_{n-2}(z), \quad q_n(z) = -\pi T_{n-1}(z), \quad z \in (-1, 1), \tag{58}$$

with the second of these equations being valid only for the points t of the integration interval $(-1, 1)$.

Then Eq. (35) gives

$$K_n(t) = \frac{\pi T_{n-1}(t)}{2(1-t^2)U_{n-2}(t)}. \tag{59}$$

Furthermore, by taking into account Eqs. (54), (55) and (56) as well as the following properties of the Chebyshev polynomials:

$$T_n'(z) = nU_{n-1}(z), \quad U_{n-1}'(z) = \frac{zU_{n-1}(z) - nT_n(z)}{1-z^2}, \tag{60}$$

from Eq. (36) we can easily find that

$$\Lambda_n(t) = -\frac{1}{4} A_m \frac{t}{1-t^2}. \tag{61}$$

Evidently, this equation is valid only for the abscissae τ_m used except the abscissae ± 1. For these particular abscissae ± 1 the Cauchy type integral (2) has no meaning as was already mentioned.

7.5. Final remarks

In this section, we considered the Gaussian numerical integration rules of open type (Gauss-type) and of closed type (Lobatto-type) associated with the Legendre and the Chebyshev polynomials. In a similar way, we can treat the cases of numerical integration rules of semi-closed type (Radau-type) associated with the same systems of orthogonal polynomials. Furthermore, we can treat the cases of numerical integration rules associated with other systems of orthogonal polynomials such as the Jacobi polynomials $P_n^{(\alpha,\beta)}(z)$, the Laguerre polynomials $L_n(z)$, the generalized Laguerre polynomials $L_n^{(\alpha)}(z)$ and the Hermite polynomials $H_n(z)$. The properties of these polynomials have been completely investigated and are mentioned in Refs. [10–12]. Finally, we can generalize an arbitrary numerical integration rule of the form (6) for regular integrals associated with a polynomial $\sigma_n(z)$ so that it can become applicable to the case of Cauchy type principal value integrals in accordance with the previous developments.

8. Examples

In this final section, we will illustrate the above results in four concrete examples.

8.1. First example

As a first example, let us consider the Cauchy type principal value integral

$$I = \fint_{-1}^{1} \frac{e^x}{x}\, \mathrm{d}x \approx 2.11450175 \tag{62}$$

also considered by Hunter [3], who applied the Gauss–Legendre quadrature rule to its evaluation. For $n = 3, 4$ and 5 the approximate values I_n of this integral obtained by using the Gauss–Legendre quadrature rule are $I_3 = 2.11449246$, $I_4 = 2.11450172$ and $I_5 = 2.11450175$, respectively [3]. Since the pole of this Cauchy type principal value integral is the point $x = 0$, the second of these values was obtained by using Eq. (33), whereas the first and the third of these values were obtained by using Eq. (34) since the point $x = 0$ is an abscissa of the Gauss–Legendre quadrature rule when n is an odd number.

For the evaluation of this integral I we can also apply the Lobatto–Legendre quadrature rule developed in the case of Cauchy type principal value integrals in the previous section. By using the same formulae, Eqs. (33) and (34), exactly as in the case of the Gauss–Legendre quadrature rule, together with Eqs. (49) and (51), for $n = 3, 4$ and 5, we find the following approximate values I_n of the aforementioned integral I: $I_3 = 2.11680080$, $I_4 = 2.11451416$ and $I_5 = 2.11450179$, respectively, which are a little less accurate than the corresponding values obtained by using the Gauss–Legendre quadrature rule. This fact is completely justified since the Gauss–Legendre quadrature rule is accurate for integrands $\phi(t)$ polynomials of degree up to $2n-1$ whereas the Lobatto–Legendre quadrature rule is accurate for integrands $\phi(t)$ polynomials of degree up to $2n-3$ [9]. In the case of Cauchy principal value integrals, the corresponding degrees of the integrands $\phi(t)$ increase by one.

8.2. Second example

As a second example, let us consider the integral

$$I(y,\lambda) = \int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} \frac{1}{(\lambda - x)(x^2+y^2)}\, \mathrm{d}x \tag{63}$$

previously considered by Paget and Elliott [13], who used a numerical integration rule developed by them for the evaluation of Cauchy type principal value integrals and based on the interpolation technique for its computation. For $y = 5$ Paget and Elliott [13] calculated the integral $I(y,\lambda)$ by the method proposed by them for $\lambda = 0.25$ and $\lambda = 0.99$. The corresponding values of the relative errors in the approximate calculations of this integral with $n = 2$ can be found from Ref. [13] to be 0.74% and 2.9%, respectively. If we use the Gauss–Chebyshev quadrature rule with $n = 2$ (which can be considered equivalent to $n = 1$ for the method of Paget and Elliott [13]) for the evaluation of the same integral $I(y,\lambda)$, Eqs. (33) and (53), the corresponding relative error is reduced to 0.019% for both values of λ. Furthermore, if we use the Lobatto–Chebyshev quadrature rule with $n = 2$, Eqs. (33) and (59), the value of the relative error is 1.9% for both values of λ. Thus it is seen that the Gauss–Chebyshev quadrature rule gives better results than both the Lobatto–Chebyshev quadrature rule and the method of Paget and Elliott [13], which is based on the interpolation technique.

8.3. Third example

As a third example, we consider the Cauchy type principal value integral

$$I(y) = \int_{0}^{1} \frac{\mathrm{d}x}{\sqrt{x}\,(x-y^2)} = \frac{1}{y} \ln \frac{1-y}{1+y}, \quad 0 < y < 1. \tag{64}$$

This integral was considered by Kutt [14]. For its approximate calculation (for $y = 0.6$) Kutt applied a complicated quadrature rule based on the splitting of the aforementioned integral $I(y)$ into three integrals followed by approximate evaluations of these integrals [14].

Here by taking into account the fact that

$$\int_{0}^{1} \frac{1}{\sqrt{\tau}}\, \phi(\tau)\, \mathrm{d}\tau = \int_{-1}^{1} \phi(t^2)\, \mathrm{d}t, \quad \tau = t^2, \tag{65}$$

for the evaluation of the integral $I(y)$ defined by Eq. (64) we can use the Gauss–Legendre quadrature rule with $2n$ abscissae, which, because of Eq. (65), in our case can be written as

$$I(y) = \sum_{k=1}^{n} A_k \frac{1}{x_k^2 - y^2} - \frac{2}{y} \frac{Q_{2n}(y)}{P_{2n}(y)}, \tag{66}$$

where x_k are the n positive abscissae of the Gauss–Legendre quadrature rule with $2n$ abscissae and A_k are the corresponding weights. Furthermore, it can easily be seen that Eq. (66) does not constitute an approximation to the integral $I(y)$, but it is exact for any value of n since, in fact, the integrand in the integral $I(y)$ defined by Eq. (64) is equal to 1. Therefore, of course, the Gauss–Legendre quadrature rule is exact. For $n = 1$ the right-hand side of Eq. (66) can easily be shown to be identical to the right-hand side of Eq. (64). This fact can also be shown for all values of n.

8.4. Fourth example

Finally, in a similar manner, we can consider the Cauchy type principal value integral

$$I^*(y) = \int_{0}^{1} \frac{\mathrm{d}x}{\sqrt{x}\,(x-y^2)^3} = \frac{3}{8y^5} \ln \frac{1-y}{1+y} + \frac{3-5y^2}{4y^2(1-y^2)^2}, \quad 0 < y < 1. \tag{67}$$

This integral, $I^*(y)$, was also computed by Kutt [14] (for $y = 0.7$) in an approximate manner exactly as the related integral $I(y)$ in Eq. (64). For the evaluation of the integral $I^*(y)$, which is a generalized integral defined in the principal value sense, Eq. (2), we can express it by a formula analogous to Eq. (66) resulting after two successive differentiations of Eq. (66) with respect to y^2. This happens simply since the integral $I^*(y)$ in Eq. (67) can be considered as resulting by two successive differentiations of the integral $I(y)$ in Eq. (64) with respect to y^2. Thus, it is possible to evaluate the integral $I^*(y)$ like the integral $I(y)$ in an exact manner by using numerical integration rules.

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