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奇异问题中奇异积分的数值方法

NUMERICAL METHOD OF SINGULAR PROBLEMS ON SINGULAR INTEGRALS

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摘　要

在许多实际问题中，需要数值计算奇异积分数值求解奇异微分方程的初、边值问题及奇异积分方程。提出的数值方法，处理了一些具有奇异被积函数的特殊函数，等离子体色散函数，第一类椭圆积分等。文中还导出了利用普通求积法计算各种奇异类型被积函数的求积公式，改善了用普通求积法计算不收敛或计算结果差的状况，特别是对多重积分计算更为显著。

NUMERICAL METHOD OF SINGULAR PROBLEMS ON SINGULAR INTEGRALS

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ABSTRACT

As first part on the numerical research of singular problems, a numerical method is proposed for singular integrals. It is shown that the procedure is quite powerful for solving physics calculation with singularity such as the plasma dispersion function. Useful quadrature formulas for some class of the singular integrals are derived. In general, integrals with more complex singularities can be dealt by this method easily.

INTRODUCTION

In various fields of physics, engienrring and other natural science, singular problems creat severe numerical difficulties on the integrals, differential equations and integral equations. Many existed numerical methods cause the divergence or slow convergence so that no any result or only poor results are obtained. More powerful methods are needed.

In this paper, we just study the singular integrals. Many important specific functions can be represented concisely by the integrals. Up to now, they cannot be integrated immediately by conventional numerical quadrature method due to their singularity, for example, the plasma dispersion function and others. In practice, the computations of these funciions with integral expression are very needful. So a variety of approximation, series expansions, continued fractions, asymptotic expansions and rational approximations are used for computing them, but some of them are complicated with slow convergence, (so that the effect is poor). Here, a numerical method is suggested, that can be used directely to integrate the singular integral without making any approximation. Numerical results show that the method is very succesful. Especially, in multiple integrals the proper treatment of singulartity play more important role due to strong singularity.

1 THE METHOD OF QUADRATURE

The computation of singular integrals can be classified into four types as following:

$$\begin{aligned} I_1 &= \int_a^b f(x)g(x)\mathrm{d}x \\ &= \int_a^b [f(x) - f(x_0)]g(x)\mathrm{d}x + f(x_0)\int_a^b g(x)\mathrm{d}x \end{aligned} \tag{1}$$

$$\begin{aligned} I_2 &= \int_a^b \frac{f(x)}{s(x)}\mathrm{d}x \\ &= \int_a^b \frac{[f(x) - f(x_0)]}{s(x)}\mathrm{d}x + f(x_0)\int_a^b \frac{1}{s(x)}\mathrm{d}x \end{aligned} \tag{2}$$

$$I_3 = \int_a^b \frac{f(x)}{s(x)}dx = \int_a^b \frac{f(x) - G(x)}{s(x)}dx + \int_a^b \frac{G(x)}{s(x)}dx \tag{3}$$

$$I_4 = \int_a^b \frac{f(x)}{s(x)}dx = \int_a^b \frac{f(x)q(x)/s(x) - f(x_0)q(x_0)/s(x_0)}{q(x)}dx + \frac{f(x_0)q(x_0)}{s(x_0)}\int_a^b \frac{1}{q(x)}dx \tag{4}$$

here $g(x) \to \infty, s(x) \to 0$ when $x \to x_0, x_0 \in [a,b]$. Set

$$F_1 = [f(x) - f(x_0)]g(x)$$

$$F_2 = [f(x) - f(x_0)]/s(x)$$

$$F_3 = [f(x) - G(x)]/s(x)$$

$$F_4 = [f(x)\, q(x)/s(x) - f(x_0)q(x_0)/s(x_0)]/q(x)$$

The following requirements are needed. (1) The $F_1(x), F_2(x), F_3(x), F_4(x)$ and $q(x)/s(x)$ tend to finite value respectively as x tends to x_0; (2) The functions of $g(x)$, $1/s(x), G(x)/s(x)$ and $1/q(x)$ with sigularities should be integrable analytically; (3) The derivative of $F_1(x), F_2(x), F_3(x)$ and $F_4(x)$, should be as finite as possible when x tends to x_0, other wise we divide the integral interval into two parts, then integrate them respectively.

The first term of right hand in (1), (2), (3) and (4) should be integrated numerically, and the second term is integrated analytically. So we can use general quadrature to integrate (1), (2), (3) and (4).

$$I_1 \approx \sum A_i F_1(x_i) + f(x_0)\int_a^b g(x)dx \tag{5}$$

$$I_2 \approx \sum A_i F_2(x_i) + f(x_0)\int_a^b \frac{1}{s(x)}dx \tag{6}$$

$$I_3 \approx \sum A_i F_3(x_i) + \int_a^b \frac{G(x)}{s(x)}dx \tag{7}$$

$$I_4 \approx \sum A_i F_4(x_i) + \frac{f(x_0)q(x_0)}{s(x_0)}\int_a^b \frac{1}{s(x)}dx \tag{8}$$

Using the formula (4) many integrals with very complex singularities can be performed by removing singularities, as long as we can choose a function $q(x)$ which is the more simple and satisfies requirements of (1), (2) and (3) listed above. For example we may choose x, x, $2x/\pi$ and ax/b as $q(x)$ when $s(x)$ are $\sin(x)$, $\exp(x)-1$, $H_0^{(x)}$ (Struve' s function) and $-1+M(a,b,x)$ (Kummer' s function) respectively. Ordinarily, the $q(x)$ can be replaced in the form of $a(x-x_0)^\beta$.

The method is sufficiently general, reatively simple, and easily applicable to singular integrals.

2 THE PLASMA DISPERSION FUNCTION

The plasma dispersion function is defined as

$$Z(s) = \pi^{-1/2}\int_{-\infty}^{\infty} \frac{\exp(-t^2)}{t-s}dt \tag{9}$$

with complex variable $s = x + iy$, $\mathrm{Im}s > 0$. It is closely related to error function $W(s)$ which is

$$W = i\pi^{-1}\int_{-\infty}^{\infty} \frac{\exp(-t^2)}{s-t}dt \tag{10}$$

$$Z(s) = i\sqrt{\pi}W(s) \tag{11}$$

This function is widely used in electromagnetic waves propagation, scatting theory of quantum mechanics, spectroscopy and plasma wave instability. The real part of $W(s)$ is called as Voigt function in astronomy. As the fuction is computed directely according to the formula (9), it is rather difficult to obtain correct result due to singularity of the function, and the math tables for this function are unsatisfied because of lack of proper procedure handling the singularity.

In order to improve computation, P. Mattin[1] has adopted four order Pade approximation instead of two order, and G. Nemeth[2] has considered two sided Pade approximation of $s=0$ and $s=\infty$. But they discuss only numerical results for real variable with low accuracy. In the same regime the results obtained by our method agree completely with the exact solution.

The plasma dispersion function is divided into real part and imaginary part

$$Z_R(s) = \pi^{-1/2}\int_{-\infty}^{\infty} \frac{t-x}{(t-x)^2+y^2}\exp(-t^2)dt \tag{12}$$

$$Z_I(z) = \pi^{-1/2}\int_{-\infty}^{\infty} \frac{y}{(t-x)^2+y^2}\exp(-t^2)dt \qquad (13)$$

The integrand of (12)has $1/(t-x)$ singularity and the integrand of (13)has Dirac delta singularity.

Utilizing

$$\int_{-\infty}^{\infty} \frac{t-x}{(t-x)^2+y^2}dt = 0$$

(12)becomes

$$Z_R = \pi^{-1/2}\int_{-\infty}^{\infty} \frac{(t-x)[1-\exp(t^2-x^2)]}{(t-x)^2+y^2}\exp(-t^2)dt \qquad (14)$$

or utilizing

$$\exp(-x^2)\int_{-\infty}^{\infty} \frac{(t-x)\cdot\exp[-(t-x)^2]}{(t-x)^2+y^2}dt$$
$$= \exp(-x^2)\int_{-\infty}^{\infty} \frac{ue^{-u^2}du}{u^2+y^2} = 0$$
$$u = t-x$$

(12)becomes

$$Z_R = \pi^{-1/2}\int_{-\infty}^{\infty} \frac{(t-x)(1-\exp(2tx-2x^2))}{(t-x)^2+y^2}\exp(-t^2)dt \qquad (15)$$

Taking account of

$$\int_{-\infty}^{\infty} \frac{1}{(t-x)^2+y^2}dt = \frac{\pi}{y}$$

(13)becomes

$$Z_I = \pi^{-1/2}\int_{-\infty}^{\infty} \frac{y(1-\exp(t^2-x^2))}{(t-x)^2+y^2}\exp(-t^2)dt + \pi^{1/2}\exp(-x^2) \qquad (16)$$

or taking advantage of

$$y\exp(-x^2)\int_{-\infty}^{\infty}\frac{\cos(t-x)}{(t-x)^2+y^2}dt = y\exp(-x^2)\pi y^{-1}\exp(-y) = \pi\exp(-x^2-y)$$

(13)becomes

$$Z_1 = \pi^{-1/2}\int_{-\infty}^{\infty}\frac{y(1-\cos(t-x)\exp(t^2-x^2))}{(t-x)^2+y^2}\exp(-t^2)dt + \pi^{1/2}\exp(-x^2-y) \quad (17)$$

There is no any singularity in the integrands of (14),(15),(16)and(17). We can use existing quadrature method to solve them.

3 THE FIRST COMPLETE ELLIPTIC INTEGRAL

First complete elliptic integral is designated as follows

$$K(m) = \int_0^{\pi/2}\frac{d\theta}{(1-m\sin^2\theta)^{1/2}} = \int_0^1\frac{dt}{[(1-t^2)(1-mt^2)]^{1/2}} \quad (18)$$

The integrand has a singularity as $m=1$. To take advantage of

$$\int\frac{dx}{(ax^2+bx+c)^{1/2}} = \frac{1}{\sqrt{a}}\log(2ax+b+2\sqrt{a}\sqrt{ax^2+bx+c}) \quad (a>0)$$

according to method of section 1,(18) can be written in

$$K(m) = \int_0^1 F(m,t)dt + \frac{1}{\sqrt{2m}}\log\frac{1+\sqrt{m}}{1-\sqrt{m}} \quad (19)$$

here

$$F(m,t) = \frac{\sqrt{1-mt}/\sqrt{(1+t)(1-mt^2)} - 1/\sqrt{2}}{\sqrt{mt^2-(1+m)t+1}}$$

4 DISCUSION

In the appendix, other quadrature formulas of the integrals with some class of singularities are derived.

It is noted that new integrand is not unique using the method described in section 1, for instance (14) and (15) for Z_R(16)and (17)for Z_I, we prefer to choose the formulas with small, rounding error i. e. choose (15)and (17)instead of using (14)and (16).

For computation of the plasma dispersion function, we use Gauss- Hermite quadrature formula when y is far from zero. (15)and (17)are adopted when y is close to zero. Using finite intergral interval the estimated error is

$$R_r = \int_R^{\infty} \frac{(t-x)\exp(-t^2)}{(t-x)^2+y^2}dt < \frac{1}{R-x}\frac{\exp(-R^2)}{R}$$

Numerical results (Table 1)show that our method is very succesful and results are more close to the exact function Z than all the others published before.

Even if integrals are very complex and hard to be solved, it is easy and convenient to calculate the integrals by using formula (4)or changing expression of the integrands properly. For instance,

$$I = \iiiint_D \frac{(R_0+x)r[1-(r/a)^a]^b}{\sqrt{(R_t+R_s)^2+Z_s-4R_tR_s\sin^2\theta}}dxd\theta drd\beta \qquad (20)$$

here $R_t = R_0 + x, R_s = R_0 + r\sin\beta, Z_s = r\cos\beta$. The integrand is singular when $R_t = R_s, Z_s = 0, \sin^2\theta = 1$. Eq. (20)can be written as

$$\begin{aligned} I &= \iiiint_D \frac{f(x,\theta,r,\beta)}{\sqrt{ar^2+br+c}}dxd\theta drd\beta \\ &= \iiiint_D \frac{f(x,\theta,r,\beta)-f(x,\theta,X,\beta)}{\sqrt{ar^2+br+c}}dxd\theta drd\beta \\ &+ \iiint f(x,\theta,X,\beta)\int\frac{dr}{\sqrt{ar^2+br+c}}dxd\theta drd\beta \qquad (21) \end{aligned}$$

here $a = 1, b = f_1(R_0,\theta,\beta,x), c = f_2(R_0,\theta,\beta,x)$. The integral $\int\frac{dr}{\sqrt{ar^2+br+c}}$ with singularity can be integrated analytically, so (21) can be integrated using the conventional quadrature method.

Table 1 Numerical Results of the Plasma Dispersion Function

	This paper		Math Table[4]	
y = 0.0				
x	Z_R	Z_I	Z_R	Z_I
0.0	0.000000E00	0.177245E01	0.000000E00	0.177245E01
0.2	−0.389502E00	0.170295E01	−0.389502E00	0.170295E01
0.4	−0.719867E00	0.151038E01	−0.719867E00	0.151038E01
0.6	−0.949526E00	0.123660E01	−0.949526E00	0.123660E01
1.0	−0.107616E01	0.652049E00	−0.107616E01	0.652049E00
2.0	−0.602681E00	0.324636E-01	−0.602681E00	0.324636E-01
4.0	−0.258696E00	0.199463E-06	−0.258696E00	0.199463E-06
6.0	−0.169006E00	0.411124E-15	−0.169006E00	0.411124E-15
y = 0.1				
x	Z_R	Z_I	Z_R	Z_I
0.0	0.000000E00	0.158927E01	0.000000E-35	0.158893E01
0.2	−0.328350E00	0.153351E01	−0.328350E00	0.153314E01
0.4	−0.610043E00	0.137796E01	−0.610043E00	0.137767E01
0.6	−0.814734E00	0.115400E01	−0.814734E00	0.115400E01
1.0	−0.954564E00	0.661442E00	−0.954564E00	0.661487E00
2.0	−0.587715E00	0.712446E-01	−0.587715E00	0.712551E-01
4.0	−0.258500E00	0.695115E-02	−0.258500E00	0.695112E-01
6.0	−0.169035E00	0.290155E-02	−0.169035E00	0.290155E-02
y = 0.2				
x	Z_R	Z_I	Z_R	Z_I
0.0	0.000000E00	0.143477E01	0.000000E-39	0.143395E-01
0.2	−0.278990E00	0.138954E01	−0.278990E00	0.138879E01
0.4	−0.522259E00	0.126283E01	−0.522259E00	0.126225E01
0.6	−0.703402E00	0.107860E01	−0.703402E00	0.107822E01
1.0	−0.848990E00	0.661434E01	−0.848990E00	0.661396E01
2.0	−0.569546E00	0.105495E00	−0.569546E00	0.105516E00
4.0	−0.257915E00	0.138672E-01	−0.257915E00	0.138672E-01
6.0	−0.168883E00	0.579773E-02	−0.168883E00	0.579774E-02
y = 1.0				
x	Z_R	Z_I	Z_R	Z_I
0.4	−0.185009E00	0.718702E00	−0.185010E00	0.715749E00
1.0	−0.369058E00	0.540343E00	−0.369058E00	0.540145E00
4.0	−0.240768E00	0.643072E-01	−0.240768E00	−0.643072E-01
8.0	−0.123084E00	0.157450E-01	−0.123084E00	0.157459E-01

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APPENDIX

Quadrature for Some Class of Singular Integrals

Quadrature formulas for some class of singular, integrals are derived according to the method of Section 1

$$\int_0^1 f(x)\ln x dx = \int_0^1 (f(x) - f(0))\ln x dx - f(0) \tag{A1}$$

$$\int_\alpha^\beta \frac{f(x)}{e^{ax} - e^{-ax}} dx = \int_\alpha^\beta \frac{f(x) - f(0)}{e^{ax} - e^{-ax}} dx + f(0) \frac{1}{2a} \ln \frac{e^{ax} - 1}{e^{ax} + 1} \Bigg|_\alpha^\beta \tag{A2}$$

$$(\alpha < 0 < \beta)$$

$$\int_\alpha^\beta \frac{f(x)}{(ax^2 + bx + c)^{3/2}} dx = \int_\alpha^\beta \frac{f(x) - f(x_0)}{(ax^2 + bx + c)^{3/2}} dx + f(x_0) I_0 \tag{A3}$$

$$I_0 = \begin{cases} -\dfrac{2(2ax + b)}{(b^2 - 4ac)\sqrt{ax^2 + bx + c}} \Bigg|_\alpha^\beta & b^2 \neq 4ac \\ -\dfrac{2\sqrt{a}}{2ax + b} \Bigg|_\alpha^\beta & b^2 = 4ac \end{cases}$$

x_0 is a root of $ax^2 + bx + c = 0$, and $\alpha < x_0 < \beta$

$$\int_\alpha^\beta \frac{f(x)}{(ax^2 + bx + c)} dx = \int_\alpha^\beta \frac{f(x) - f(x_0)}{(ax^2 + bx + c)} dx + f(x_0) I_0 \tag{A4}$$

Here

$$I_0 = \begin{cases} \dfrac{1}{\sqrt{b^2 - 4ac}} \ln \dfrac{2ax + b - \sqrt{b^2 - 4ac}}{2ax + b - \sqrt{b^2 - 4ac}} \Bigg|_\alpha^\beta & (b^2 > 4ac) \\ \dfrac{2}{\sqrt{b^2 - 4ac}} \operatorname{arctg} \dfrac{2ax + b}{\sqrt{4ac - b^2}} \Bigg|_\alpha^\beta & (b^2 < 4ac) \\ -\dfrac{2}{2ac + b} \Bigg|_\alpha^\beta & (b^2 = 4ac) \end{cases}$$

x_0 is a root of $ax^2 + bx + c = 0$, and $\alpha < x_0 < \beta$

$$\int_\alpha^\beta \frac{f(x)}{(ax^2+bx+c)^{1/2}}dx = \int_\alpha^\beta \frac{f(x)-f(x_0)}{(ax^2+bx+c)^{1/2}}dx + f(x_0)I_0 \quad \text{(A5)}$$

Here

$$I_0 = \begin{cases} \frac{1}{\sqrt{a}}[\ln(2ax+b+2\sqrt{a}\sqrt{ax^2+bx+c}]\Big|_\alpha^\beta & (a > 0) \\ \frac{1}{\sqrt{a}}\arcsin\frac{-2ax-b}{\sqrt{b^2-4ac}}\Big|_\alpha^\beta & (a < 0) \end{cases}$$

x_0 is a root of $ax^2 + bx + c = 0$ and $\alpha < x_0 < \beta$ 。

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