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Generalised Functions and Divergent Integrals

B. W. NINHAM

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Abstract. A method is given for the interpretation of a class of divergent integrals in terms of a sum of function evaluations over an arbitrary partition of the integration interval. The class of integrands considered includes functions continuous on the integration interval, except at a finite number of algebraic or algebraico-logarithmic singularities, and the delta function and related generalised functions, or products of these. The interpretation assigned to such integrals coincides with that of generalised function theory. Possible applications of the method to the computation of functions are discussed.

1. Introduction

In this paper we shall develop a method for the interpretation of a particular class of divergent integrals in terms of the familar idea of a limit sum. The method follows from a simple and natural extension of the Riemann integral, and the interpretation given to a divergent integral coincides with results of generalised function theory in the form presented by LIGHTHILL [1] in his book. Through the now familiar notion of a "regular sequence of good functions" TEMPLE [2] and later LIGHTHILL [1] have developed an eminently satisfactory theory distinguished by its simplicity and power. However, the theory of TEMPLE suffers from one minor disadvantage in applications to numerical work; that its intimate connection with the concept of a Riemann integral as a limit sum is not exhibited explicitly and on an elementary level. The approach to divergent integrals and generalised functions advocated here aims to exhibit this connection explicitly.

The method applies to divergent integrals of functions which are continuous on the integration interval, except at a finite number of algebraic or algebraico-logarithmic singularities. We shall also admit the delta function and related generalised functions as acceptable functions to which our interpretation of an integral applies, but exclude specifically at this stage functions with essential singularities on the integration interval. This limitation is not too restrictive, and applies equally to the work of LIGHTHILL [1].

Before launching into too much detail, we first discuss some of the typical problems which we have in mind. Consider the convergent integral

$$I f = \int_0^1 f(t)\, dt = \int_0^1 t^{\alpha}(1-t)^{\beta}\, dt = \frac{\alpha!\,\beta!}{(\alpha+\beta+1)!} \tag{1.1}$$

The integral is defined only for $\operatorname{Re}\alpha > -1$, $\operatorname{Re}\beta > -1$. Suppose that we wished to evaluate the integral using a numerical quadrature formula, which we shall call a rule, and for simplicity let us use a mid-point trapezoidal rule. Then we have

$$\int_0^1 f(t)\, dt \cong \frac{1}{m}\sum_{j=1}^{m} f(t_j) \equiv R^{[m,0]} f, \tag{1.2}$$

where

$$t_j = \frac{2j-1}{2m}; \qquad j = 1, 2, \ldots, m. \tag{1.3}$$

In making the approximation Eq. (1.2) we commit some error Ef, and can write precisely

$$If = R^{[m,0]}f - Ef \tag{1.4}$$

where (cf. NINHAM and LYNESS [3])

$$Ef = \sum_{\substack{r=-\infty \\ r\neq 0}}^{\infty} (-1)^r \int_0^1 e^{2\pi i r m t} f(t)\, dt. \tag{1.5}$$

For large m, the error term has the asymptotic expansion (NAVOT [4], and LYNESS and NINHAM [3]).

$$\begin{aligned} Ef = -\Big\{ & \frac{\zeta(-\alpha)(1-2^{-\alpha})}{m^{\alpha+1}} - \alpha \frac{\zeta(-\alpha-1)}{m^{\alpha+2}} (1-2^{-\alpha-1}) + \\ & + \frac{\alpha(\alpha-1)}{m^{\alpha+3}} \zeta(-\alpha-2)(1-2^{-\alpha-2}) + O\left(\frac{1}{m^{\alpha+4}}\right) + \\ & + - \left\{ \frac{\zeta(-\beta)}{m^{\beta+1}} (1-2^{-\beta}) - \beta \frac{\zeta(-\beta-1)}{m^{\beta+2}} (1-2^{-\beta-1}) + \cdots \right\} \end{aligned} \tag{1.6}$$

If we use this expansion for Ef in conjunction with Eq. (1.2) we obtain a very much better approximation to the integral for a given number m of function evaluations, than would be given by the rough integration rule Eq. (1.2). Further, and this is the point we wish to make, we can use Eq. (1.4) with Ef given by Eq. (1.6) to compute the integral even if it diverges ($\operatorname{Re}\alpha < -1$ and or $\operatorname{Re}\beta < -1$). The quantity computed turns out to be $\alpha!\,\beta!/(\alpha+\beta+1)!$

Again, consider the generalised zeta function, defined for $\operatorname{Re} s > 1$, and $0 < a < 1$, by

$$\zeta(s, a) = \sum_{n=0}^{\infty} \frac{1}{(n+a)^s} \tag{1.7}$$

If we use the Euler Maclaurin summation formula, we have

$$\zeta(s, a) = \frac{1}{2a^s} + \frac{a^{1-s}}{(s-1)} + \frac{1}{12}\frac{s}{a^{s+1}} - \frac{1}{720}\frac{s(s+1)(s+2)}{a^{s+3}} + \cdots \tag{1.8}$$

an asymptotic expansion which may be used to compute this function even when $\operatorname{Re} s < 1$, so that the formal series representing $\zeta(s, a)$ is divergent. For example, taking $a = 1$, so that Eq. (1.7) reduces to the ordinary zeta function, we have by direct substitution in Eq. (1.8) the well-known results

$$\zeta(0) = -\tfrac{1}{2}; \qquad \zeta(-1) = -\tfrac{1}{12}, \qquad \zeta(-2) = 0 \tag{1.9}$$

and the residue at the pole of $\zeta(s, a)$ at $s = 1$ is unity.

A variety of problems in theoretical physics and numerical analysis lead to divergent integrals and series of them types, whose manipulation to obtain correct results is not well understood.

2. Divergent Integrals as Limit Sums

With these problems in mind, we begin this investigation with a generalisation of Poisson's summation formula [3]. This formula asserts that for every Riemann integrable function $f(t)$.

$$\int_0^1 f(t)\,dt = \sum_{j=1}^{m} a_j f(t_j) - Ef \tag{2.1}$$

where the error term Ef is given by

$$Ef = \sum_{j=1}^{m} a_j \sum_{\substack{r=-\infty \\ r\neq 0}}^{\infty} \int_0^1 f(t)\, e^{2\pi i r(t-t_j)}\,dt. \tag{2.2}$$

The value of the integer m, the $t_j's$, and $a_j's$, are all arbitrary except for the normalisation condition

$$\sum_{j=1}^{m} a_j = 1 \tag{2.3}$$

and the conditions

$$0 \leqq t_j \leqq 1. \tag{2.4}$$

The identity Eq. (2.1) can be verified by integrating Eq. (2.2) twice by parts, and carrying out the sums.

We use this identity to interpret the integral on the left hand side in terms of a sum over each and every partition of the integration interval [0, 1] and an error term associated with this partition. For simplicity we shall use for the most part in the sequel a mid point trapezoidal rule given by the choice

$$t_j = \frac{2j-1}{2m}, \qquad j = 1, 2, \ldots, m; \qquad a_j = \frac{1}{m} \tag{2.5}$$

This is a convenient choice, but unnecessary, and we emphasise that the analysis goes through for an arbitrary partition, with weights a_j also arbitrary except for the normalisation condition Eq. (2.3). Then Eq. (2.1) reduces to the form

$$\int_0^1 f(t)\,dt = \frac{1}{m}\sum_{j=1}^{m} f(t_j) - 2\sum_{r=1}^{\infty} (-1)^r \int_0^1 f(t)\cos 2\pi r m t\,dt. \tag{2.6}$$

We note that

$$\begin{aligned} \lim_{m\to\infty} \frac{1}{m}\sum_{j=1}^{m} f(t_j) &= \int_0^1 f(t)\,dt; \\ \lim_{m\to\infty} Ef &= 0 \end{aligned} \tag{2.7}$$

and either Eq. (2.1) or (2.6) coincides with the usual definition of a Riemann Integral, when $f(t)$ is Riemann integrable.

We now set up a corresponding interpretation of a divergent integral, and for definiteness consider the simple example

$$I(\alpha) = \int_0^1 t^\alpha\,dt, \tag{2.8}$$

where α may be real or complex. From this integral we can develop an interpretation for any integral of a function, continuous on the integration interval except at a finite number of algebraic singularities.

For $\operatorname{Re}\alpha > -1$, we have

$$I(\alpha) = \frac{1}{(\alpha+1)}. \tag{2.9}$$

The integral $I(\alpha)$ diverges for $\operatorname{Re}\alpha < -1$, and Eq. (2.8) has no meaning in this region of the α plane. However it does have a meaning for real α; $\alpha < -1$ in generalised function theory which interprets the integral as (cf. LIGHTHILL [*1*]).

$$I(\alpha) = \int_{-\infty}^{\infty} t^{\alpha}[H(t) - H(1-t)]\,dt = \frac{1}{\alpha+1} \tag{2.10}$$

where $H(t)$ is the step function, and the generalised function $H(t)\,t^{\alpha}$ is defined as

$$t^{\alpha} H(t) = \frac{1}{(\alpha+1)(\alpha+2)\ldots(\alpha+n)}\,\frac{d^n}{dt^n}\,t^{\alpha+n} H(t) \tag{2.11}$$

where n is any integer such that $\alpha+n > -1$. The result Eq. (2.10) is the Hadamard "finite" part of the divergent integral, which is identical with the analytic continuation of Eq. (2.9) to the region $\operatorname{Re}\alpha < -1$. But this interpretation does not show explicitly the connection of such a divergent integral with the idea of a limit sum. To do this, we first use Eq. (2.6) to define $I(\alpha)$ for $-1 < \operatorname{Re}\alpha < 0$ and for every partition n. Thus we have

$$I(\alpha) = \int_0^1 t^{\alpha}\,dt = \frac{1}{m}\sum_{j=1}^{m} t_j^{\alpha} - 2\sum_{r=1}^{\infty}(-1)^r \int_0^1 \cos 2\pi r m t\, t^{\alpha}\,dt. \tag{2.12}$$

For $\operatorname{Re}\alpha < -1$ neither the integral, nor the error term on the right hand side exist. However the first term on the right hand side of Eq. (2.12) does exist, and is an analytic function of α for all α, and all finite m. If we then analytically continue the error term to the region $\operatorname{Re}\alpha < -1$, the right hand side will exist in this region, and can be used to obtain an expression for $I(\alpha)$, $\operatorname{Re}\alpha < -1$, which coincides with $1/\alpha+1$, the analytic continuation of the Riemann integral defined in $\operatorname{Re}\alpha > -1$. This programme once carried out, is at first sight nothing more than a most extraordinarily complicated method for analytically continuing the function $1/\alpha+1$. However, it does give an interpretation of the integral in terms of a sum of function evaluations over an arbitrary partition. Further, generalised functions such as the delta function are also automatically and very simply handled by this prescription.

In order to effect the analytic continuation we write

$$E f = E_1 f - E_2 f \tag{2.13}$$

where

$$E_1 f = 2\sum_{r=1}^{\infty}(-1)^r \int_0^{\infty} \cos(2\pi r m t)\, t^{\alpha}\,dt \tag{2.14}$$

and

$$E_2 f = 2\sum^{\infty}(-1)^r \int_1^{\infty} \cos 2\pi r m t\, t^{\alpha}\,dt. \tag{2.15}$$

For $-1 < \operatorname{Re}\alpha < 0$, we can carry out the integration over t and the summation over r in Eq. (2.14) to obtain

$$E_1 f = 2\sum_{r=1}^{\infty}(-1)^r \alpha!\,\frac{\cos\frac{1}{2}\pi(\alpha+1)}{(2\pi r m)^{\alpha+1}} = -\frac{2}{(2\pi m)^{\alpha+1}}\,\alpha!\cos\tfrac{1}{2}\pi(\alpha+1)\,\tau(\alpha+1) \quad (2.16)$$

where

$$\tau(s)=\sum_{r=1}^{\infty}\frac{(-1)^{r-1}}{r^s};\quad \operatorname{Re}s>0;\quad \tau(s)=(1-2^{1-s})\,\zeta(s); \quad (2.17)$$

Using the Riemann relation linking $\zeta(s)$ with $\zeta(1-s)$,

$$2^{1-s}(s-1)!\,\zeta(s)\cos(\tfrac{1}{2}s\pi)=\pi^s\zeta(1-s) \quad (2.18)$$

and the relation

$$(2^s-1)\,\zeta(s)=\zeta(s,\tfrac{1}{2}) \quad (2.19)$$

where $\zeta(s,\frac{1}{2})$ is a generalised zeta function, $E_1 f$ can be cast into the form

$$E_1 f = m^{-\alpha-1}\zeta(-\alpha,\tfrac{1}{2}). \quad (2.20)$$

Except at the single pole of the generalised zeta function at $\alpha=-1$, this is an analytic function of α, which analytically continues $E_1 f$, originally defined only for $-1<\operatorname{Re}\alpha<0$, to the region $\operatorname{Re}\alpha<-1$. We can handle the second part of the error term, Eq. (2.15), as follows. Integrating by parts twice, we have

$$\begin{aligned}E_2 f = {} & 2\frac{\alpha\,\tau(2)}{(2\pi m)^2} - 2\frac{\alpha(\alpha-1)(\alpha-2)}{(2\pi m)^4}\tau(4) + 2\frac{\alpha(\alpha-1)(\alpha-2)(\alpha-3)}{(2\pi m)^4}\times \\ & \times\sum_{r=1}^{\infty}\frac{(-1)^r}{r^4}\int_1^{\infty}\cos(2\pi r m t)\,t^{\alpha-4}\,dt.\end{aligned} \quad (2.21)$$

The first two terms of Eq. (2.23) are analytic functions of α for all α. It is a straightforward matter to show that for $\operatorname{Re}\alpha<0$ the last term is a sum of analytic functions and that the sum is uniformly convergent with respect to α, so that this term is also an analytic function of α in the region $\operatorname{Re}\alpha<0$. Collecting together Eqs. (2.12), (2.14), (2.15), (2.20) and (2.21) we have then

$$\begin{aligned}I(\alpha) = {} & \frac{1}{m}\sum_{j=1}^{m}t_j^{\alpha} - m^{-\alpha-1}\zeta\left(-\alpha,\frac{1}{2}\right) \\ & -2\left\{\frac{\alpha\,\tau(2)}{(2\pi m)^2} - \frac{\alpha(\alpha-1)(\alpha-2)\,\tau(4)}{(2\pi m)^4} + \frac{\alpha(\alpha-1)(\alpha-2)(\alpha-3)}{(2\pi m)^4}\times\right. \\ & \left.\times\sum_{r=1}^{\infty}\frac{(-1)^r}{r^4}\int_1^{\infty}\cos 2\pi r m t\, t^{\alpha-4}\,dt\right\}\end{aligned} \quad (2.22)$$

The expression on the right hand side of Eq. (2.29) is now an analytic function of α for all $\operatorname{Re}\alpha<0$, except for the single pole of the zeta function. We use it to give a meaning to the divergent integral on the left hand side, which is thereby given an interpretation in terms of a sum over an arbitrary partition. To *compute* the divergent integral exactly, we must now take the limit $m\to\infty$, just as for a convergent integral. The terms in curly brackets on the right hand side of

Eq. (2.22) disappear in the limit. The sum over j can be evaluated as follows. Since

$$\frac{1}{m}\sum_{j=1}^{m} t_j^{\alpha} = m^{-\alpha-1}\sum_{j=1}^{m}\frac{1}{(j-\frac{1}{2})^{-\alpha}} = m^{-\alpha-1}\zeta\left(-\alpha,\frac{1}{2}\right) - \frac{1}{m}\sum_{k=0}^{\infty}\frac{1}{\left(1+\frac{k+\frac{1}{2}}{m}\right)^{-\alpha}} \tag{2.23}$$

we have

$$\begin{aligned}\int_0^1 t^{\alpha}\,dt &= \lim_{m\to\infty}\left\{\frac{1}{m}\sum_{j=1}^{m} t_j^{\alpha} - \zeta\left(-\alpha,\frac{1}{2}\right)m^{-\alpha-1} - 2\left\{\frac{\alpha\,\tau(2)}{(2\pi m)^2} + O\left(\frac{1}{m^4}\right)\right\}\right\}\\ &= \lim_{m\to\infty} -\frac{1}{m}\sum_{k=0}^{\infty}\frac{1}{\left(1+\frac{k+\frac{1}{2}}{m}\right)^{-\alpha}} = \frac{1}{(\alpha+1)}\,.\end{aligned} \tag{2.24}$$

The last sum has been carried out using the Euler-Maclaurin summation formula which is certainly applicable as the sum converges, when $\operatorname{Re}\alpha < -1$.

Although we have used a special partition of the integration interval; $t_j = \frac{2j-1}{2m}$, $a_j = 1/m$, the same result would have been obtained for an arbitrary partition subject to the restrictions Eq. (2.3) and (2.4). An end point rule ($t_1 = 0$) introduces a minor complication in that an infinity at $t_1 = 0$ occurs in $\sum_{j=1}^{m} a_j t_j^{\alpha}$ for $\alpha < 0$, but this is cancelled exactly by a corresponding term in Ef. We discuss the appropriate necessary modifications in the analysis in an appendix. We note that the first two terms of the expression in curly brackets of Eq. (2.22) are the leading terms of an asymptotic expansion in the variable $1/m^2$. Further terms can be obtained by integrating by parts successively the integrals of Eq. (2.22). The fact that an asymptotic series occurs on the right hand side of the defining Eq. (2.22), whose accuracy is here strictly prescribed by the least term in this series, is a natural result. It is simply a statement that the integral, divergent or not, cannot be computed to arbitrary accuracy using a finite partition of the integration interval. Modifications of the integrand due to integral powers of logarithms can easily be handled by differentiation of the right hand side of Eq. (2.22). Thus we can write down directly from Eq. (2.22) an interpretation of the divergent integrals

$$\int_0^1 t^{\alpha}\ln t\,dt = \frac{\partial}{\partial\alpha}\int_0^1 t^{\alpha}\,dt\,. \tag{2.25}$$

3. The Singular Case

The special cases

$$I(1) = \int_0^1 \frac{dt}{t};\ \int_0^1 \frac{\ln t\,dt}{t};\ \int_0^1 \frac{dt\,f(t)\,dt}{t} \tag{3.1}$$

where $f(t)$ is analytic at $t=0$ require special attention. It was already obvious a priori that this must be so, since the analytic continuation of $\frac{1}{\alpha+1}$ does not exist at $\alpha=-1$. This is reflected naturally also in the theory of generalised functions as presented by LIGHTHILL [1], who shows that the generalised functions $|x|^{-1}$, $|x|^{-1}\operatorname{sgn} x$, $|x|^{-1}H(x)$ can be defined consistently only up to an arbitrary constant which is a multiple of the delta function. Again expressions such as $\int_0^1 dt/t^\beta$, $\int_0^1 dt/t^n$, where n in an integer $n>1$, and $\beta>1$, if interpreted according to our procedure can be shown to obey the usual rules of Riemann integration theory such as transformation of variable and integration by parts. But integration by parts or formal substitutions such as $t=x^\alpha, e^x$, sin x etc. applied to integrals like Eq. (3.1) lead back to the same singularity.

Via our approach, Eq. (2.22) shows that this difficulty is intimately related to the pole of the generalised zeta function at $\alpha=-1$. Since the generalised zeta function is analytic everywhere except at this pole, no such difficulty arises with any other value of α. In generalised function theory the functions $|x|^{-n}$, $|x|^{-n}\operatorname{sgn} x$, $|x|^{-n}H(x)$ are defined only up to an additive constant which is a constant times a derivative of the delta function.

4. Further Improper Integrals

One can use the procedure we have developed to interpret improper divergent integrals like $\int_0^1 t^\alpha F(t)\,dt$ where $\alpha<-1$, and $F(t)$ is a "good" function. We use the term "good" function in the sense of LIGHTHILL's definition — a good function is one which is everywhere differentiable any number of times, and such that it and all its derivatives are $O(|t|^{-n})$ as $|t|\to\infty$ for all n. In generalised function theory the integral is interpreted as

$$\begin{aligned}\int_0^1 t^\alpha F(t)\,dt &= \frac{(-1)^n}{(\alpha+1)(\alpha+2)\dots(\alpha+4)}\int_0^1 t^{\alpha+n}F^{(n)}(t)\,dt + \\ &+ \frac{F(1)}{(\alpha+1)} - \frac{1}{(\alpha+1)(\alpha+2)}F'(1) + \cdots + \\ &+ \frac{(-1)^{n-1}}{(\alpha+1)(\alpha+2)\dots(\alpha+n)}F^{(n-1)}(1)\end{aligned} \tag{4.1}$$

where n is the least integer for which $(\alpha+n)>-1$. Eq. (4.1) is what the ordinary formula for repeated integration by parts would give formally, if all the contributions from the lower limit, which are infinite, were omitted. Such an interpretation follows naturally, once $\int_0^1 t^\alpha dt$; $\alpha<-1$ is defined as in section 2. For then

$$\begin{aligned}\int_0^1 t^\alpha F(t)\,dt &= \int_0^1 t^\alpha\left[F(0)+tF'(0)+\frac{t^2}{2!}F''(0)+\frac{t^{n-1}}{(n-1)!}F^{(n-1)}(0)\right]dt + \\ &+\int_0^1 t^\alpha\left\{F(t)-\left[F(0)+tF'(0)+\frac{t^2}{2!}F''(0)+\frac{t^{n-1}}{(n-1)!}F^{(n-1)}(0)\right]\right\}dt.\end{aligned} \tag{4.2}$$

The first integral is divergent, and must be interpreted as in section 2. The second is an ordinary Riemann integral. We have, by Eq. (2.24)

$$\begin{aligned}\int_0^1 t^\alpha F(t)\,dt &= \frac{F(0)}{\alpha+1}+\frac{F'(0)}{(\alpha+2)}+\cdots\frac{F^{(n-1)}(0)}{(\alpha+n)(n-1)!} + \\ &+\int_0^1 t^\alpha\left\{F(t)-\left[F(0)+\frac{tF'(0)}{1!}+\cdots\frac{t^{n-1}}{(n-1)!}F^{(n-1)}(0)\right]\right\}dt.\end{aligned} \tag{4.3}$$

Successive integration by parts of the convergent integral which remains on the right hand side, and rearrangement, gives the interpretation Eq. (4.1). We note that this interpretation coincides with the analytic continuation of $\int_0^1 t^\alpha F(t)\,dt$, defined for $\operatorname{Re}\alpha > -1$ to the region $\operatorname{Re}\alpha < -1$. More generally it is sufficient that $F(t)$ be differentiable any number of times in some interval which includes $(0, 1)$, because any such function necessarily coincides with some good function in $(0, 1)$. That $F(t)$ must necessarily be a good function follows from the requirement that the interpretation Eq. (4.1) hold for all α. If $F(t)$ is not a good function, and contains several algebraic or algebraico-logarithmic singularities, it is sufficient to divide the integration range into several each of which contains only a single singularity, and proceed as above.

5. Delta and Related Functions

The delta function of Dirac can be defined in a variety of ways, each involving a limiting process. Thus for example we may define

$$\delta(x) = \lim_{n\to\infty} \frac{n}{\sqrt{\pi}} e^{-\frac{x^2}{n^2}}, \tag{5.1}$$

$$\delta(x) = \frac{1}{2\pi} \lim_{k\to\infty} \int_{-k}^{k} e^{itx}\,dt, \tag{5.2}$$

or

$$\delta(x) = \frac{1}{\pi} \lim_{\sigma\to 0} \left(\frac{\sigma}{x^2+\sigma^2}\right). \tag{5.3}$$

Each has the property that

$$\int_{-\infty}^{\infty} \delta(t) F(t)\,dt = F(0) = \int_a^b F(t)\,\delta(t)\,dt; \qquad b > 0 > a \tag{5.4}$$

provided that $F(t)$ is a good function. In order to demonstrate this propertly via our approach, we consider the integral

$$I = \int_0^1 dt \frac{F(t)}{(t^2+\sigma^2)} \tag{5.5}$$

We shall be interested in $\lim\limits_{\sigma\to} \frac{\sigma I}{\pi}$, where I is interpreted as a sum over every partition m of the interval $[0, 1]$ and an error term. From Eq. (2.6) we have, for every m

$$I = \frac{1}{m}\sum_{j=1}^{m} (t_j^2+\sigma^2)^{-1} F(t_j) - \sum_{r=-\infty}^{\infty} (-1)^2 \int_0^1 \frac{e^{2\pi i r m t}}{(t^2+\sigma^2)} F(t)\,dt \tag{5.6}$$

where again, we use a mid-point rule for convenience only $\left(a_j = \frac{1}{m},\ t_j = \frac{2j-1}{2m}\right)$. As in section 2 we write the error term Ef as

$$Ef = E_1 F - E_2 F \tag{5.7}$$

where

$$E_1F = 2\sum_{r=1}^{\infty}(-1)^2\int\limits_0^{\infty}\frac{\cos(2\pi r m t)}{(t^2+\sigma^2)}F(t), \tag{5.8}$$

$$E_2F = 2\sum_{r=1}^{\infty}(-1)^2\int\limits_1^{\infty}\frac{\cos(2\pi r m t)}{(t^2+\sigma^2)}F(t)\,dt \tag{5.9}$$

and $F(t)$ must be such that each of the integrals converge. For large m, and small σ successive integration by parts in Eq. (5.9) shows immediately that

$$E_2F = O\left(\frac{1}{m^2}\right). \tag{5.10}$$

We shall obtain an appropriate expansion for the term E_1F by the following technique. The integral representation

$$\frac{1}{t^2+\sigma^2} = \frac{1}{2\pi i}\int\limits_{c-i\infty}^{c+i\infty}(p-1)!\,(-p)!\,\frac{(\sigma^2)^{p-1}}{t^{2p}}\,dp; \qquad 0<\operatorname{Re}p<1 \tag{5.11}$$

after substitution in Eq. (5.9) allows us to write

$$E_1F = \frac{2}{2\pi i}\int\limits_{c-i\infty}^{c+i\infty}(p-1)!\,(-p)!\,(\sigma^2)^{p-1}\sum_{r=1}^{\infty}(-1)^r\int\limits_0^{\infty}\cos 2\pi r m t\, t^{-2p}F(t)\,dt. \tag{5.12}$$

We write

$$\begin{aligned}\int\limits_0^{\infty}\cos 2\pi r m t F(t)\,t^{-2p}\,dt = &\int\limits_0^{\infty}\cos 2\pi r m t F(0)\,t^{-2p}\,dt + \\ &+\int\limits_0^{\infty}\cos 2\pi r m t[F(t)-F(0)]\,t^{-2p}\,dt\end{aligned} \tag{5.13}$$

and substitute into Eq. (5.12). Remembering that we are interested in the limit $\sigma\to 0$, it is not difficult to show that the second integral will go to zero as $\sigma\ln\sigma$, so that we drop it forthwith. Retaining only the first integral of Eq. (5.13), and using the relation

$$\int\limits_0^{\infty}\cos 2\pi r m t\, t^{-2p}\,dt = \frac{1}{(2\pi r m)^{1-2p}}(-2p)!\cos\left[\frac{\pi}{2}(1-2p)\right], \qquad 0<\operatorname{Re}p<\tfrac{1}{2} \tag{5.14}$$

we have, after carrying out the sum over t,

$$\begin{aligned}E_1F = &\frac{-2}{2\pi i}\int\limits_{c-i\infty}^{c+i\infty}(p-1)!\,(-p)!\,\sigma^{2p-2}\frac{\tau(1-2p)}{(2\pi m)^{1-2p}}(-2p)!\times \\ &\times\cos\frac{\pi}{2}(1-2p)\,F(0), \qquad 0<\operatorname{Re}p<\tfrac{1}{2}\end{aligned} \tag{5.15}$$

If we close the contour of integration to the right, the first contributing pole of the integrand is that of $(-2p)!$ at $p=\frac{1}{2}$, with residue $-\frac{1}{2}$, and we find

$$\begin{aligned}E_1F &= -2\sigma^{-1}\pi\frac{\tau(0)}{2}F(0) + O(m^2) \\ &= \frac{-\pi}{2\sigma}F(0) + O(\sigma m^2)\end{aligned} \tag{5.16}$$

since $\tau(0)=\frac{1}{2}$. Hence finally

$$\begin{aligned}\frac{\sigma}{\pi} I &= \frac{\sigma}{\pi}\int_0^1 dt \frac{F(t)}{(t^2+\sigma^2)} \\ &= \frac{\sigma}{\pi m}\sum_{j=1}^{m}(t_j^2+\sigma^2)F(t_j)+\frac{F(0)}{2}+O(\sigma m^2)+O(\sigma\ln\sigma).\end{aligned} \tag{5.17}$$

This representation is to hold for every partition m. Taking the limit $\sigma\to 0$ first, and *after* the limit $m\to\infty$, we have

$$\lim_{\sigma\to 0}\frac{\sigma}{\pi}\int_0^1 dt\frac{F(t)}{t^2+\sigma^2}=\int_0^1 \delta(t)F(t)\,dt=\frac{F(0)}{2} \tag{5.18}$$

This corresponds with the usual result for

$$\int_0^1 \delta(t)F(t)\,dt=\frac{F(0)}{2} \tag{5.19}$$

Further we can use the method developed above to construct more complicated generalised functions. For example, the functions, and their derivatives

$$\delta_\alpha(t)=\lim_{\sigma\to 0}\frac{1}{\pi_\sigma}\left(\frac{\sigma^2}{t^2+\sigma^2}\right)^\alpha; \qquad \operatorname{Re}\alpha>\tfrac{1}{2} \tag{5.20}$$

of which the delta function of a Dirac is a special case with

$$\delta_1(t)=\delta(t) \tag{5.21}$$

can be shown by the above technique to have the property that

$$\int_0^1 \delta_\alpha(t)F(t)\,dt=\frac{1}{\sqrt{\pi}}\frac{(\alpha-3/2)!}{(\alpha-1)!}\frac{F(0)}{2} \tag{5.22}$$

6. Application to Computation of Functions

Very many of the functions which turn up in mathematical physics have simple integral representations for some values of the defining parameters. For example the confluent hypergeometric functions, which include the Bessel, parabolic cylinder functions, exponential integrals and related functions, some orthogonal polynomials, and many others, have the integral representation

$$\Phi(a,c,x)=\frac{(c-1)!}{(a-1)!\,(c-a-1)!}\int_0^1 e^{xt}t^{a-1}(1-t)^{c-b-1}\,dt; \qquad \operatorname{Re}c>\operatorname{Re}a>0. \tag{6.1}$$

Similarly the hypergeometric functions have in standard notation the integral representation

$$F(a,b;c;z)=\frac{(c-1)!}{(b-1)!\,(c-b-1)!}\int_0^1 t^{b-1}(1-t)^{c-b-1}(1-tz)^{-a}\,dt; \qquad \operatorname{Re}c>\operatorname{Re}b>0. \tag{6.2}$$

For values of the parameters a, b, c, for which these integrals converge, these functions can be computed in terms of a sum of function evaluations (or integration rule), and a remainder. Asymptotic expansions for the remainder or error term associated with any integration rule have been developed in an earlier series of papers [3]. These expansions apply to integrals of functions whose singularities in the complex integration plane are either non-essential, or whose essential singularities are sufficiently far removed from the integration axis. For any such integral, the error incurred in using a particular partition of the integration interval can be written down by inspection, and the methods developed combine the some of the better features of numerical and analytic techniques.

The analysis of the preceding sections, with minor and straightforward extensions, shows that the same expansions can also be used for values of the parameters for which the integrals diverge. The divergent integral computed in this manner gives the analytic continuation of the function, defined by an ordinary Riemann integral for some ranges of the defining parameters. The sole difference from the point of view of numerical analysis, is that the leading terms of the "error term" associated with a given integration rule sometimes dominate. The roles of the error and integration rule are thereby reversed.

As a simple numerical example, consider the integral of Eq. (1.1)

$$I(\alpha, \beta) = \int_0^1 t^\alpha (1-t)^\beta \, dt = \frac{\alpha!\, \beta!}{(\alpha+\beta+1)!} \tag{6.3}$$

where I exists as an ordinary convergent integral for $\operatorname{Re}\alpha > -1$, $\operatorname{Re}\beta > -1$. Our prescription should yield this result for all α and β. For convenience we take $\alpha = -\frac{3}{2}$, $\beta = -\frac{3}{2}$, and using the expansion Eq. (1.6) we have

$$I(-\tfrac{3}{2}, -\tfrac{3}{2}) \equiv 0 = \int_0^1 t^{-\frac{3}{2}} (1-t)^{-\frac{3}{2}} \, dt = Rf - Ef \tag{6.4}$$

with

$$R = \frac{1}{m} \sum_{j=1}^{m} f(t_j); \tag{6.5}$$

$$\begin{aligned} E = -2\Big\{ & \zeta\left(+\tfrac{3}{2}\right)\left(1 - 2^{\frac{3}{2}}\right) m^{\frac{1}{2}} + \tfrac{3}{2}\zeta\left(\tfrac{1}{2}\right)\left(1 - 2^{\frac{1}{2}}\right) m^{-\frac{1}{2}} + \\ & + \frac{(\frac{3}{2})(\frac{5}{2})}{2!}\zeta\left(-\tfrac{1}{2}\right)\left(1 - 2^{-\frac{1}{2}}\right) m^{-\frac{3}{2}} + \cdots \Big\} \end{aligned} \tag{6.6}$$

In the worst possible situation — a one point integration rule ($m = 1$), we have

$$\begin{aligned} E = -2\{ & -4.7765\,3802 + 0.9073\,4827 - 0.1141\,6693 - 0.0360\,3870 + \\ & + 0.172\,5460 + 0.0010\,6260 - 0.0008\,6669 - 0.000\,8207 + \\ & + 0.000\,9069 + \text{increasing terms}\}. \end{aligned} \tag{6.7}$$

Truncating the asymptotic series at its least term we have

$$E = -8.0030, \qquad R = 8, \qquad I = 0.003.$$

For other values of m, the rate at which the successive terms in the asymptotic series for E decrease is vastly improved. Thus for $m=8$ we have, truncating the series at its 5^{th} term, beyond which succeeding terms are negligible

$$R=26.389051\,; \qquad E=-26.389052; \qquad I=0.000001\,,$$

the error here being due to round off in R.

In so far as numerical stability is concerned, it is clear that the utility of expansions such as Eq. (6.7) are not markedly different whether associated with either convergent or divergent integrals. Since one would normally choose by inspection of the appropriate asymptotic expansions for $E f$ — the *least* possible value of m consistent with a prescribed accuracy — the circumstance that R and E are sometimes of comparable magnitude for divergent integrals is not usually important — except in so far as one must compute the first one or two zeta functions with high accuracy. But this in itself of course presents no problem. The example we have chosen is one of the worst one could imagine, since we are computing a quantity which is identically zero, and any instability should certainly show up. It would seem that numerical instability will arise in the particular case of integrands with singularities on the integration interval — of very high order, e.g. of the type t^α; $|t-\gamma|^\alpha \operatorname{sgn}(t-\gamma)$; $t^\alpha \ln|t|$; $|t-\gamma|^\alpha \ln|t-\gamma| \operatorname{sgn}(t-\gamma)$ where $|\alpha|$ is very large. However this instability is common to both convergent and divergent integrals, and seems to be connected ultimately with the circumstance that one of the simplest of functions, a very high degree polynomial, is in general difficult to compute with ease.

Appendix

Behaviour near Rule Singularity

We investigate here the behaviour of the generalised Poisson summation formula, used in section 2 to define a divergent integral in terms of a sum over an arbitrary partition, if the partition uses a point for function evaluations at which the function becomes infinite. We consider again, so as not to obscure the underlying simplicity of the analysis the integral

$$I(\alpha)=\int_0^1 t^\alpha\,dt \tag{A.1}$$

and use a trapezoidal rule given by

$$a_j=\frac{1}{m}, \qquad t_j=\frac{j+\delta-1}{m}\,; \qquad j=1,2,\ldots m. \tag{A.2}$$

For $-1<\alpha<0$, the integral (A.1) certainly exists as a Riemann integral and can be defined in terms of a sum over the partition (A.2) by the generalised Poisson summation formula as

$$\int_0^1 t^\alpha\,dt=\frac{1}{m}\sum_{j=1}^{m} t_j^\alpha-\frac{1}{m}\sum_{\substack{r=-\infty\\ r\neq 0}}^{\infty}\sum_{j=1}^{m}\int_0^1 t^\alpha e^{2\pi i r(t-t_j)}\,dt. \tag{A.3}$$

We are interested in the behaviour of the right hand side as $\delta \to 0+$, when the first term of the rule, $t_1 = (\delta/m)^\alpha$ diverges. Since

$$\sum_{j=1}^{m} e^{-2\pi i r t} j = e^{-\frac{-2\pi i r}{m}(\delta-1)} \frac{1}{m} \sum_{j=1}^{m} e^{\frac{-2\pi i r}{m} j} = \begin{cases} 0; & r \neq \text{multiple of } m \\ e^{2\pi i r\left(\frac{\delta-1}{m}\right)}; & r = \text{multiple of } m \end{cases} \tag{A.4}$$

we can write the error term of Eq. (A.3) as

$$E = \sum_{\substack{r=-\infty \\ r \neq 0}}^{\infty} e^{-2\pi i r \delta} \int_0^1 t^\alpha e^{2\pi i r t m} \, dt$$

$$= 2 \sum_{r=1}^{\infty} \int_0^1 t^\alpha \cos 2\pi r (m t - \delta) \, dt = E_1 - E_2 \tag{A.5}$$

where

$$E_1 = 2 \sum_{r=1}^{\infty} \int_0^{\infty} t^\alpha (\cos 2\pi r m t \cos 2\pi r \delta + \sin 2\pi r m t \sin 2\pi r \delta) \, dt, \tag{A.6}$$

$$E_2 = 2 \sum_{r=1}^{\infty} \int_1^{\infty} t^\alpha \cos 2\pi r (m t - \delta) \, dt. \tag{A.7}$$

We can find a convenient expansion for E_2 by integrating by parts, and find

$$\begin{aligned} E_2 = 2 \sum_{r=1}^{\infty} \bigg\{ & \frac{\sin 2\pi r \delta}{2\pi r m} + \alpha \frac{\cos 2\pi r \delta}{(2\pi r m)^2} - \\ & - \frac{1}{(2\pi r m)^2} \int^{\infty} \cos 2\pi r (m t - \delta) \, \alpha (\alpha - 1) \, t^{\alpha-2} \, dt \bigg\}. \end{aligned} \tag{A.8}$$

The first two sums are simply Bernoulli polynomials in δ, apart from factors $1/m$, α, and the last sum can easily be shown to be an analytic function of α, m, and δ for all $\operatorname{Re} \alpha < 0$. As $\delta \to 0+$, Eq. (A.8) reduces to the form

$$E_2(\delta = 0) = 2 \left[\frac{\alpha}{(2\pi m)^2} \zeta(2) - \frac{\alpha(\alpha-1)(\alpha-2)}{(2\pi m)^4} \zeta(4) + O\left(\frac{1}{m^6}\right) \right] \tag{A.9}$$

Carrying out the integrals over t in Eq. (A.6) we have

$$E_1 = 2 \sum_{r=1}^{\infty} \frac{\alpha!}{(2\pi r m)^{1+\alpha}} \left\{ \cos \frac{\pi}{2} (\alpha + 1) \cos 2\pi r \delta + \sin 2\pi r \delta \sin \frac{\pi}{2} (\alpha + 1) \right\} \tag{A.10}$$

We can carry out the sums over r as follows. Writing

$$\cos 2\pi r \delta = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{(p-1)!}{(2\pi r \delta)^p} \cos \frac{\pi}{2} p \quad 0 < \operatorname{Re} p < 1, \tag{A.11}$$

$$\sin 2\pi r \delta = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{(p-1)! \sin \frac{\pi}{2} p}{(2\pi r \delta)^p} \quad -1 < \operatorname{Re} p < 1 \tag{A.12}$$

and substituting in Eq. (A.10), we can interchange orders of integration and summation to find

$$E_1 = \frac{2}{m^{1+\alpha}}\,\alpha!\,\frac{1}{2\pi i}\int\limits_{c-i\infty}^{c+i\infty}(p-1)!\sum_{r=1}^{\infty}\times$$

$$\times\frac{\left[\cos\frac{\pi}{2}(\alpha+1)\cos\frac{\pi}{2}p+\sin\frac{\pi}{2}(\alpha+1)\sin\frac{\pi}{2}p\right]}{(2\pi r)^{1+\alpha+p}\,\delta^p}\,dp; \tag{A.13}$$

$$= \frac{2\alpha!}{m^{1+\alpha}}\,\frac{1}{2\pi i}\int\limits_{c-i\infty}^{c+i\infty}(p-1)!\,\frac{\left(-\sin\frac{\pi}{2}\alpha\cos\frac{\pi}{2}p+\cos\frac{\pi}{2}\alpha\sin\frac{\pi}{2}p\right)}{(2\pi)^{1+\alpha+p}\,\delta^p}\,\zeta(1+p+\alpha)\,dp -$$

$$-\alpha<\operatorname{Re}p<1.$$

Closing the contour of integration to the left, we have

$$E_1 = \frac{2\alpha!}{m^{1+\alpha}}\left\{\frac{(-\alpha-1)!\sin\pi\alpha}{2\pi\,\delta^{-\alpha}}+\frac{\cos\frac{\pi}{2}\alpha}{(2\pi)^{1+\alpha}}\zeta(1+\alpha)+O(\delta)\right\} \tag{A.14}$$

$$= \frac{\delta^\alpha}{m^{1+\alpha}}+2\alpha!\,\frac{\cos(\pi/2)\,\zeta(1+\alpha)}{(2\pi m)^{1+\alpha}}+O(\delta). \tag{A.15}$$

This function is an analytic function of δ, $\delta\neq 0$ and an analytic function of α for all $\alpha<0$. For all $\alpha<0$, we have then

$$\int\limits_0^1 t^\alpha\,dt = \frac{1}{m}\sum_{j=1}^{m}t_j^\alpha-\left[\frac{\delta^\alpha}{m^{1+\alpha}}+2!\,\frac{\cos\frac{\pi}{2}\alpha\,\zeta(1+\alpha)}{(2\pi m)^{1+\alpha}}+O(\delta)\right]+ \\ +2\left[\frac{\alpha\,\zeta(2)}{(2\pi m)^2}-O\left(\frac{1}{m^4}\right)+O(\delta)\right]. \tag{A.16}$$

As $\delta\to 0$, we see that the term in the rule for which $j=1$, cancels exactly a corresponding term of the error expansion. When the rest of the sum is performed as in section 2 we recover the result $I(\alpha)=1/\alpha+1$.

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The University of New South Wales
School of Mathematics
P.O. Box 1
Kensington, N.S.W., Australia