Numerical integration in many dimensions. I

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If a d-dimensional integral involves an integrand of the functional form $F(f_1(x_1) + f_2(x_2) + \cdots)$, then one can introduce an integral transform (Fourier or Laplace or variants on those) which allows all the integrals over the coordinates x_i to factor. Thus a d-dimensional integral is reduced to a one-dimensional integral over the transform variable. This is shown to be a very powerful and practical numerical approach to a number of problems of interest. Among the examples studied is the computation of the volume of phase space for an arbitrary collection of relativistic particles. One important aspect of the approach involves numerical integration along various contours in the complex plane.

I. INTRODUCTION

If an accurate numerical evaluation of a one-dimensional integral requires n points on a lattice, then, according to conventional wisdom, one will require n^d lattice points to evaluate a similar d-dimensional integral. This number n^d grows so rapidly as d increases that such a direct approach becomes prohibitive. Thus there has been great interest in Monte Carlo and related methods that appear to be independent of the number of dimensions. This paper reports an attempt to turn against this tide and to find some analytically based schemes for multidimensional integration that have high accuracy and systematic improvement with considerably less than n^d operations.

In Sec. II, I consider integrals that involve a function (or a few functions) of the form $F(f_1(x_1) + f_2(x_2) + \cdots + f_d(x_d))$. An integral transform is used to reduce the d-dimensional integral to a one-dimensional (or a few-dimensional) integral over the transform variable(s). An interesting aspect of this method is that one often ends up integrating numerically over some contour in the complex plane; and some examples show that this can be done quite nicely. This method is applied to computation of the relativistically invariant phase space volume for any number of particles with arbitrary masses and some total energy specified in Sec. III.

In Sec. IV, I consider integrands F whose argument is a product, rather than a sum, of functions of the different variables. Here a Mellin transform does the trick; and some further examples are given.

The philosophy guiding this work is not that one should expect a universal rule good for all types of functions. Rather, the aim is to develop a variety of techniques, each one powerful for certain classes of functions. Then, either through analysis or by trial and error, one can seek the procedure most efficient for any given problem. While the particular type of function studied in this paper may seem very special, it appears to be the most commonly encountered in studies of multidimensional integrals and is familiar in many physics problems.

In the following paper[1] two very different new techniques for multidimensional integration are presented.

II. THE TRANSFORM METHOD

Consider integrals of the form

$$I = \left(\prod_{i=1}^{d} \int g_i(x_i)dx_i\right) F\left(\sum_{i=1}^{d} f_i(x_i)\right). \tag{1}$$

Assume that we can find a suitable integral transform for the function F:

$$F(s) = \int d\sigma\, \hat{F}(\sigma) e^{su(\sigma)}; \tag{2}$$

then the original integral becomes

$$I = \int d\sigma\, \hat{F}(\sigma) \prod_{i=1}^{d} w_i(\sigma), \tag{3}$$

where

$$w_i(\sigma) = \int g_i(x)dx\, e^{f_i(x)u(\sigma)}. \tag{4}$$

Thus we have replaced a d-dimensional integral by $(d+1)$ one-dimensional integrals. This implies a great economy: from n^d to $n^2 d$ operations.

The choice of the integral representation (2) will depend on the nature of the function F and the range of the variables. Some examples:

$$\theta(s) s^{p-1} = \int_{C-i\infty}^{C+i\infty} \frac{d\sigma}{2\pi i} \frac{\Gamma(p)}{\sigma^p} e^{s\sigma}, \quad p>0; \tag{5}$$

$$s^{-p} = \int_0^\infty d\sigma \frac{\sigma^{p-1}}{\Gamma(p)} e^{-s\sigma}, \quad p>0, \quad s>0. \tag{6}$$

These can be used as in the following d-dimensional integrals:

$$\left(\prod_{i=1}^{d} \int_0^\infty dx_i\, x_i^{\alpha_i - 1} e^{-\beta_i x_i}\right)\left(\sum_{i=1}^{d} x_i + \gamma\right)^{p-1} = \int_{C-i\infty}^{C+i\infty} \frac{d\sigma}{2\pi i} \frac{\rho(p)}{\sigma^p} e^{\gamma\sigma} \prod_{i=1}^{d} \frac{\Gamma(\alpha_i)}{(\beta_i - \sigma)^{\alpha_i}}, \quad 0<C<\beta_i \tag{7}$$

and

$$\left(\prod_{i=1}^{d} \int_0^1 dx_i\right)\left(\sum_{i=1}^{d} a_i x_i + a_0\right)^{-p} = \int_0^\infty d\sigma \frac{\sigma^{p-1}}{\Gamma(p)} e^{-\sigma a_0} \prod_{i=1}^{d} \left(\frac{1-e^{-a_i\sigma}}{a_i\sigma}\right). \tag{8}$$

After one has chosen an integral transform the final task is to select a good contour and to have a reliable scheme for numerical integration. It is well known that one can make this last task terribly hard by choosing an unfortunate contour for integration—one where the function is very large and rapidly oscillating so that numerical accuracy is rapidly lost. However, (as is perhaps less well known) con-

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tour integration in the complex plane can also be a very easy and well-behaved problem.

For a test I chose the representation of the gamma function given in (5):

$$\frac{1}{\Gamma(p)} = \int_{C-i\infty}^{C+i\infty} \frac{d\sigma}{2\pi i}\frac{e^{\sigma}}{\sigma^{p}}. \tag{9}$$

If you look at the integrand along the positive real axis, you see that it has a minimum at $\sigma = p$. Furthermore, if σ can go to infinity in the left half-plane, then the exponential will decay rapidly. So I chose the contour

$$\sigma = p + 1 - \cosh x + i \sinh x, \quad -\infty < x < \infty. \tag{10}$$

Finally, for the infinite integration over x, I use the simple rule

$$\int_{-\infty}^{\infty} f(x)dx \cong h \sum_{n=-\infty}^{\infty} f(x_0 + nh), \tag{11}$$

which will generally have an error decreasing exponentially fast with decreasing h, for analytic functions f (see Ref. 2). Results of this computation are given in Table I; they look quite satisfactory. I redid the computation with the alternative contour

$$\sigma = p + i \sinh x \tag{12}$$

and found that the results were about the same for large values of p but for smaller p the integration required more points to be taken for the same accuracy. (For $p = 2$ it did not work at all.) This carries the interesting lesson that some problems may get *easier* as the number of dimensions gets larger: Note the increasing number of powers of σ in the denominators of (7) and (8) as d increases; and it is this large negative exponent that helps make the final integral converge rapidly in a small domain.

TABLE I. Numerical integration for the gamma function $\Gamma(p)$. Results from the equation $1/\Gamma(p) = \int_{C-i\infty}^{C+i\infty} (d\sigma/2\pi i)(e^{\sigma}/\sigma^{p})$, with integration along the contour $\sigma = p + 1 - \cosh x + i \sinh x$ are given. The trapezoidal rule was used for integration in x, terminating when the added terms were less than one part in 10^7. The machine was accurate to six decimal figures of arithmetic. The interval h was started at 1.0 and then successively halved. The numbers in parentheses give the number of integration points used at each value of h. This could have been reduced by half by using the symmetry in x. The dot under each number indicates the place after which it ceases to be accurate.

$p = 2$		$p = 16$		$\times 10^{-13}$
0.993 299	(9)	0.111 804	(9)	
1.000 461	(15)	0.128 573	(17)	
1.000 002	(29)	0.130 805	(30)	
		0.130 767	(57)	
$p = 4$		$p = 32$		$\times 10^{-34}$
6.572 09	(9)	1.851 694	(9)	
6.006 62	(15)	0.918 359	(17)	
6.000 00	(27)	0.820 985	(33)	
		0.822 279	(63)	
$p = 8$		$p = 64$		$\times 10^{-88}$
4605.07	(9)	0.145 196	(11)	
4985.79	(15)	0.208 250	(19)	
5039.94	(28)	0.198 967	(37)	
5040.00	(53)	0.198 261	(71)	

Sometimes this integral transform technique allows one to express a complicated-looking multidimensional integral in closed form. For example, in Eq. (7), if p should be an integer or if the numbers α_i are integers, then one can write the answer in terms of residues at the poles at $\sigma = 0$ or $\sigma = \beta_i$ (for $\gamma = 0$.) A large number of multidimensional integrals of this general type have been evaluated by Fichtenholz[3] using more laborious techniques. I prefer to stress the practicality of numerical integration as illustrated here rather than struggling for "closed form" answers.

As an illustration of this last remark consider the integral

$$\int_{-\infty}^{\infty} dx\, x^2 \prod_{i=1}^{N} \frac{\sin p_i x}{p_i x}, \tag{13}$$

which was derived by Cerulus and Hagedorn[4] by an integral transform from some other multidimensional integral. Those authors showed how to evaluate this algebraically in 2^N operations by means of residues. (Sometimes this involves much cancellation between nearly equal terms. The entire integral vanishes if any one p exceeds the sum of the others.) I tried integrating (13) directly, using the rule (11), and found that it worked excellently, except for very small N.

III. PHASE SPACE INTEGRAL

I have applied this method to an interesting and difficult problem which has long concerned high-energy physicists: calculating the volume of phase space for N particles with total energy E. The relativistically invariant integral is expressed in momentum variables as

$$R_N = \left(\prod_{i=1}^{N} \int \frac{d^3 p_i}{2E_{p_i}}\right) \delta^3\left(\sum_i \mathbf{p}_i\right) \delta\left(\sum_i E_{p_i} - E\right), \tag{14}$$

where

$$E_{p_i} = +(\mathbf{p}_i^2 + m_i^2)^{1/2}. \tag{15}$$

I start by introducing the Fourier integral representation of the Dirac delta functions,

$$\delta^3(\mathbf{p})\delta(E) = \int \frac{d^3x\, dt}{(2\pi)^4} e^{i\mathbf{p}\cdot\mathbf{x}} e^{-iEt}, \tag{16}$$

and then we have the separate integrals over each momentum variable which result in the modified Bessel function of order 1:

$$\int \frac{d^3 p}{2E_p} e^{i\mathbf{p}\cdot\mathbf{x}} e^{-iE_p t} = 2\pi \frac{m}{(\mathbf{x}^2 - t^2)^{1/2}} K_1(m\sqrt{\mathbf{x}^2 - t^2}). \tag{17}$$

From (17) we see that the integration variable t may be taken into the lower half of the complex plane; this means that the square root expression $(\mathbf{x}^2 - t^2)^{1/2}$ always has a positive real part. Now we introduce a new integration variable σ as follows. Writing for shorthand

$$\Pi(\sigma) = \prod_{i=1}^{N} \frac{2\pi m_i}{\sigma} K_1(m_i \sigma), \tag{18}$$

the integral (14) is equal to

$$R_N = \int \frac{d^3x\, dt}{(2\pi)^4} \int_{C-i\infty}^{C+i\infty} d\sigma\, \Pi(\sigma) \frac{i\sigma/\pi}{\sigma^2 - \mathbf{x}^2 + t^2} e^{+iEt}, \tag{19}$$

where C is a small positive constant so that the contour runs to the right of the singularity at $\sigma = 0$ and to the left of the poles at $\sigma = (\mathbf{x}^2 - t^2)^{1/2}$. Now the integrals over $\mathbf{x}$ and t can be carried out, giving us another Bessel function; and the final result is

$$R_N = \frac{1}{4\pi^2 i}\int_{C-i\infty}^{C+i\infty} d\sigma \frac{\sigma^2}{E} I_1(\sigma E)\Pi(\sigma). \qquad (20)$$

Thus the $3N$-[or ($3N$-4)-] dimensional integral (14) is transformed into a single integral (20). A few analytic remarks can be made before proceeding to discuss the numerical evaluation of this integral.

The contour of integration may be moved about since now the only singularity of the integrand occurs at the origin. If we move far to the right, the Bessel functions can be replaced by their asymptotic forms and we have the simple exponential behavior

$$\exp(E-M): \quad M = \sum_{i=1}^{N} m_i. \qquad (21)$$

Thus if E is less than M, the integral is seen to vanish, which is physically correct. If the masses of the particles are all zero, we have

$$\frac{m_i}{\sigma} K_1(m_i\sigma) \rightarrow \frac{1}{\sigma^2}, \qquad (22)$$

and the integral becomes

$$R_N(0) = \frac{1}{4\pi i^2}\int_{C-i\infty}^{C+i\infty} d\sigma \frac{I_1(\sigma E)}{E}\frac{(2\pi)^N}{\sigma^{2N-2}}, \qquad (23)$$

which can be evaluated in terms of the pole at the origin, yielding the well-known result

$$R_N(0) = (\pi/2)^{N-1} E^{2N-4}/(N-1)!(N-2)!. \qquad (24)$$

The nonrelativistic limit is gotten by taking the masses of the particles large and using the asymptotic formulas for the Bessel functions:

$$(m_i/\sigma)K_1(m_i\sigma) \rightarrow (m_i\pi/2\sigma^3)^{1/2} e^{-m_i\sigma}, \qquad (25)$$

$$I_1(\sigma E) \rightarrow (1/2\pi E\sigma)^{1/2} e^{\sigma E}, \qquad (26)$$

$$R_N \rightarrow \left(\prod_{i=1}^{N} m_i^{1/2}\right)\frac{1}{E^{3/2}} \pi^{(3/2)(N-1)} 2^{(1/2)(N-3)} \times \frac{1}{2\pi i}\int_{C-i\infty}^{C+i\infty} d\sigma \frac{e^{(E-m)\sigma}}{\sigma^{(3/2)(N-1)}}, \qquad (27)$$

and the final integral is given by (5). Hybrid closed forms, where some of the particles are considered ultrarelativistic according to (22) and the rest are treated nonrelativistically according to (25) and (26), can also be obtained. As far as I am aware, such closed form results for (14) are new.[5]

For numerical evaluation of (20) we first choose the contour, following the earlier experience with the similar, but much simpler integral (9). Along the real axis, the integrand in (20) grows large at both small σ and large σ; so we shall choose the contour through the point $\sigma = C$ where the integrand has its minimum. Upper and lower bounds for C can be well estimated by using the approximation (26) for the function I_1 and either of the approximations (22) or (25) for the functions K_1:

$$C = [(2 - \tfrac{1}{2}\zeta)N - \tfrac{3}{2}]/(E-M), \qquad (28)$$

where

$$0 < \zeta < 1.$$

In my program I let the machine choose the minimum point after three evaluations of the integrand: at the two extremes of (28) and at their midpoint.

Next is the question of how to evaluate the Bessel functions occurring in the integrand (20). I used the polynomial approximations for I_1 and K_1 given by Abramowitz and Stegun.[6] These have an advertised accuracy of about one part in 10^7 or better for *real* arguments; one could worry about their accuracy for the complex arguments needed in our integral. However, I was able to convince myself that this procedure was adequate for the present uses. Finally, there is the task of the actual numerical integration. I used the simple rule (11) after a change of variables

$$\sigma = C(1 + ixe^{x^2}), \qquad (29)$$

which helps the integrand to decrease rapidly. Working to an accuracy of one part in 10^4 for the final answer I found that as few as 15 points in the numerical integration were required for large values of N (20 or more); about 40 points were needed at $N = 6$ and about 160 at $N = 3$. The program did not work for $N = 2$. I have ideas about how to change the contour so that this could be improved but it hardly seemed worthwhile. Small-N results can be calculated directly from (14) much more simply. The hard problem is for large N and here my program worked beautifully.

A few checks on the program are available. The zero-mass result (24) is one. The case of all but one particle having mass zero is another[7]; and the case of three particles of equal mass m is given by the integral [gotten directly from (14)]

$$2(1-3\gamma)^2(1+\gamma)^2 \int_0^1 dx \times \left[x(1-x)\frac{(1+3\gamma)(1-\gamma)-(1-3\gamma)(1+\gamma)x}{4\gamma^2+(1-3\gamma)(1+\gamma)x}\right]^{1/2} \qquad (30)$$

where

$$\gamma = m/E,$$

and this is normalized to unity at $\gamma = 0$.

A production run for ten values of N (from $N = 3$ to $N = 30$) and nine values of M/E (from 0 to 0.5) took about 10 s of computer time and cost just over one dollar. This was for the case of all masses equal so that each Bessel function K was evaluated only once at each integration point. In general the time required will be proportional to the number of different masses; but this should still be far far less than the time for any other known method at large N.

A summary of the calculated results (for N equal mass particles) is

$$\rho_N = R_N(m)/R_N(0) \cong \rho_2 e^{-\lambda(N-2)}, \quad \rho_2 = (1-(M/E)^2)^{1/2}, \quad M = Nm, \qquad (31)$$

and the value of λ is given by

$$\lambda \cong (M/E)^2 \ln(E/M)^2, \qquad (32)$$

for small values of M/E (up to 0.1) and increases to about twice this value at $M/E = 0.5$.

IV. ANOTHER TRANSFORM USED

Multidimensional integrals that have the particular form (1) might be thought of as being terribly special. Yet, if one looks at the leading textbook on numerical integration[8] this is the most common form of examples shown. Out of a total of 26 numerical examples given by Davis and Rabinowitz for integrals in more than two dimensions, 16 are of the form (1); and all but one of the remaining examples are of the alternate form:

$$J=\left(\prod_{i=1}^{d}\int g_i(x_i)dx_i\right)F\left(\prod_{i=1}^{d}f_i(x_i)\right). \tag{33}$$

The change from a sum to a product in the argument of the function F leads us to use a Mellin transform in order to factorize the dependence on the separate coordinates x_i. The transform is

$$F(t)=\int_{C-i\infty}^{C+i\infty}\frac{d\sigma}{2\pi i}t^{-\sigma}\hat{F}(\sigma), \tag{34}$$

and its inverse is

$$\hat{F}(\sigma)=\int_0^\infty dt\,F(t)t^{\sigma-1}. \tag{35}$$

This leads to the single integral for J, analogous to (3),

$$J=\int\frac{d\sigma}{2\pi i}\hat{F}(\sigma)\prod_{i=1}^{d}w_i(\sigma), \tag{36}$$

where

$$w_i(\sigma)=\int dx\,g_i(x)[f_i(x)]^{-\sigma}. \tag{37}$$

One example of reduction of a d-dimensional integral of this form is

$$\left(\prod_{i=1}^{d}\int_0^1 dx_i\,x_i^q\right)F\left(\prod_{i=1}^{d}x_i\right)=\int_0^1 dt\,t^qF(t)\frac{[\ln 1/t]^{d-1}}{(d-1)!}. \tag{38}$$

A second example is

$$\prod_{i=1}^{d}\left(\int_0^\infty dx_i\,e^{-x_i}\right)\exp\left(-b\prod_{i=1}^{d}x_i\right)=\int\frac{d\sigma}{2\pi i}\Gamma(\sigma)\Gamma^d(1-\sigma)b^{-\sigma}, \tag{39}$$

which involves gamma functions, entering as the Mellin transform of the exponential function. The contour of integration here is parallel to the imaginary axis, passing between the poles at $\sigma=0$ and $\sigma=1$. Numerical evaluation of (39) was carried out very successfully, following the general advice given in Sec. II. Gamma functions for complex argument are readily computed by starting with the general asymptotic expansion for moderately large argument. For $d=10$ and various values of b $(2,10,100,2i,10i,100i)$ I was able to obtain six-figure accuracy with under 100 integration points.

Other examples, both analytical and numerical, were studied but need not be recorded here.

V. FURTHER REMARKS

The general technique described here may be of particular practical use in some statistical problems. If one has several independent random variables x_i, distributed according to probability functions $g_i(x_i)$, then an integral of the form (1) with $F=\delta(R-\Sigma_{i=1}^d x_i)$ gives the probability distribution for the sum of the variables to have the value R. Some previous work on such problems, it appears, could benefit from the present technique.[9]

In conclusion I should note some possible extensions of the method of integral transforms described above. If the multidimensional integral has not just one function F of the form shown in (1) but a few of them in product, then one could carry out an integral transform (2) for each of them. The resulting product integral in the transform variables might still be more tractable by direct integration than was the original integral.

If an analytic expression for the transform $\hat{F}$ is not available, one might evaluate this also by numerical integration of the inverse transform of F. Similarly, if the integrals w_i of (4) do not give nice closed form answers, numerical integration may be used on these one-dimensional integrals. Thus, for the Bessel functions of complex argument needed in the phase space problem, one could get them directly by numerical integration from the integral representations for these Bessel functions. (I have tried this and it works well.)

Finally, if the function F is of the form $F(f_{12}(x_1,x_2)+f_{34}(x_3,x_4)+\cdots)$, there is an obvious generalization of the method that might be useful.

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