JOURNAL OF COMPUTATIONAL PHYSICS 3, 512–522 (1969)

Variational Principles for Integrals[1]

CHARLES SCHWARTZ

Department of Physics and Lawrence Radiation Laboratory
University of California, Berkeley, California 94720

Received October 2, 1968

ABSTRACT

We consider the problem of approximating integrals of the form $\int 1/W$ where W may be a simple (e.g. polynomial) form in the integration variables. A variational expression is given which approximates this integral in terms of integrals of W with suitably chosen trial functions. The power of this method is compared with that of Gaussian quadrature in a few examples. Some generalizations of the method are discussed.

INTRODUCTION

Calculations in quantum field theory are usually carried out in terms of the perturbation theory expansion, where each term is represented by a Feynman diagram. This diagram is a mnemonic for writing down a multidimensional integral over the momenta of the intermediate particles. While much attention in the literature has been given to deriving these rules and analysing the formal properties of the integrals involved, there has not been much study of how to get numbers out of this formalism beyond the lowest order terms. The problem is not trivial for two reasons. First is the high dimensionality of the integrals: a three loop diagram may represent a Feynman-parametrized integral with eight variables. If our integration formula needs n points per dimension to get the required accuracy and we have d dimensions, then we need a total of $N = n^d$ evaluations of the integrand. While in one, two, or even three dimensions the capacity of modern computing machines lets us use standard methods with many points, as we go to higher dimensionality it becomes imperative to have a small number n of points per dimension.

High accuracy with a small number of integration points means we must have some sophisticated rule for numerical integration, and this brings us to the second hurdle: For any cookbook rule of numerical integration (Simpson's rule, Gauss

[1] This work was supported in part by the U.S. Atomic Energy Commission.

quadrature, etc., etc.) the advertised accuracy depends on the assumed analytic smoothness of the integrand. Thus consider an integral over the unit interval: with Simpson's rule and n points we are told the error goes as

$$n^{-4} \text{ times the } 4\text{th derivative of the function,}$$

and for the n point Gaussian formula the error goes approximately as

$$n^{-2n} \text{ times the } 2n\text{th derivative of the function.}$$

If the higher derivatives of the integrand are bounded these methods will produce results which improve rapidly in accuracy as the number of points increases. However, if the integrand has even some mild singularity, a higher derivative will be unbounded and the fancier integration formulas may work no better than cruder ones. Ultimately the development of accurate numerical integration formulas for a given problem requires a careful study of the singularities of that particular function; so the practical problem of evaluating Feynman integrals will relate to the esoteric study of the singularities of these integrals which has been in vogue lately.

What makes this problem complicated from a numerical analysis point of view is that the singularities are not associated with just the individual coordinates but lie on various hypersurfaces in a many dimensional space. Take for example the integral

$$\int_0^1 ds \int_0^1 dt \, \frac{1}{(s+t)} ;$$

this is easy enough to do analytically, but I challenge anyone to show me a standard method which works at all efficiently. (A change of variables is not allowed since it is not part of a standard method but part of the artist's skill, to be used differently with each new problem.) In the present paper we present one new method which has been found in thinking about this general sort of problem.

The Variational Method

The simplest type of integral to do is a polynomial form; the type we want to consider here involves a quotient of polynomial forms. For shorthand we will write the single variable x for whatever set of variables x_1, x_2,..., we are given; and

$$\int dx$$

for the multidimensional integral over some specified domain in the many variables. We study the integral

$$I = \int dx \, \frac{\rho(x)}{W(x)}, \tag{1}$$

and with a further simplifications of notation write

$$\int \quad \text{for} \quad \int dx \rho(x);$$

then

$$I = \int \frac{1}{W}. \tag{2}$$

Variational principles have been used in the solution of algebraic, differential and integral equations; we will now write down a variational principle for the evaluation of the integral I. Define the functional

$$J = 2 \int \phi - \int \phi W \phi. \tag{3}$$

Its variation with respect to the function ϕ is

$$\delta J = 2 \int \delta\phi [1 - W\phi] \tag{4}$$

which vanishes if $\phi = 1/W$ at all points x within the integral. The stationary value of J is then

$$J(\phi = 1/W) = \int 1/W = I. \tag{5}$$

One can use this principle as follows. Choose a function ϕ which has some of the general features as $1/W$ but simpler in detail so that the integrals $\int \phi$ and $\int \phi W \phi$ can be evaluated. (Note that W instead of its inverse is involved here.) Then vary some parameters in ϕ to make J stationary. If ϕ differs from $1/W$ by some small error of measure ϵ, then J will differ from I in measure ϵ^2.

$$J\left(\phi = \frac{1}{W} + \Delta\right) = I - \int \Delta W \Delta. \tag{6}$$

This shows that if the weight function ρ and W are everywhere positive, the error has a definite sign: J is a lower bound to I.

The most convenient way to vary constants is to make a linear expansion of ϕ in some convenient set of basis functions $u_n(x)$. With

$$\phi = \sum_n C_n u_n \tag{7}$$

we need for J the matrix elements

$$M_{nn'} = \int u_n W u_{n'} \tag{8}$$

and the vector components

$$r_n = \int u_n . \tag{9}$$

This gives from the stationary conditions

$$\frac{\delta J}{\delta C_n} = 0 \tag{10}$$

the linear algebraic equations

$$\sum_{n'} M_{nn'} C_{n'} = r_n \tag{11}$$

and the answer

$$I \approx \sum_{n} C_n r_n . \tag{12}$$

This solution can be written in the vector and matrix language as

$$I \approx r \cdot M^{-1} \cdot r. \tag{13}$$

Here we see the inverse of the matrix M giving us the inverse of the function W for the original integral.

This method looks like a lot of work: In order to do one integral we must first evaluate many integrals—(8) and (9)—and then do some matrix algebra. The linear algebra is a standard computing machine function; the choice of the basis functions u_n is up to the artist. One should choose functions u_n so that the required integrals can be readily tabulated by the computer; however bear in mind that these functions u_n are trying to represent an expansion of the function $1/W$, and one will want to have the general shape and some analytic properties of $1/W$ represented in these basis functions if this expansion is to converge rapidly. In any calculation we will truncate the expansion at some size, say N, and the error will then be something proportional to the square of the magnitude of the next neglected coefficient in the complete expansion.

Before going into some examples it is interesting to make a comparison of this approach with the general Gaussian technique [1]. The integral

$$\int f(x)\, dx \tag{14}$$

is represented by the sum

$$\sum w_i f(x_i). \tag{15}$$

The n points x_i and the n weights w_i are to be chosen so that the representation is exact for some chosen set of $2n$ functions $v_j(x)$. i.e.,

$$\int v_j = \sum_{i=1}^{n} w_i v_j(x_i); \qquad j = 1, 2n. \tag{16}$$

Here are $2n$ nonlinear equations to be solved for the $2n$ unknowns w_i and x_i before the method can be used to evaluate some integral of interest; and in order to set up these equations we must first do the $2n$ integrals of the chosen functions v_j. If the given function $f(x)$ were expanded in an infinite series of the basis functions v_j, the error in the use of the nth order formula (15) for the integral (14) would be proportional to the expansion coefficient for the first neglected function, of order $2n$.

We can see several similarities between our method and the Gauss method, they may in general be considered to be fair competitors. The possible disadvantage of the variational method is the greater family of integrals which one must evaluate first to build the matrix; the possible disadvantage of the Gauss method is the nonlinear search for the points x_i in Eq. (16). (This nonlinear problem is not very difficult to handle in the classical cases where $v_j = v_0 x^{j-1}$.) Aside from the question of labor, the accuracies are given by the smallness of the expansion coefficient C_{2n} on the one hand, and the square, $(C_n)^2$, on the other hand. For a geometric convergence

$$C_n \sim a^n \qquad (a < 1) \tag{17}$$

these two estimates are equal; for any faster convergence the Gaussian method looks better, for any slower convergence the variational method looks better. Just what the convergence of the expansion will be in any given case may be found by a comparison of the analytic properties of the expansion functions, u or v, with the function they are trying to represent, $1/W$ or f.

Now we report some examples.

Example 1.

$$I_1 = \int_0^1 ds s(2s - 1)/(1 - s + s^2). \tag{18}$$

We take $W = (1 - s + s^2)$, and absorb the numerator factor into the symbol $\int$. Within the region of integration $1/W$ is analytic and so we take for ease of integration

$$u_n = s^{n-1} \qquad n = 1, 2, \ldots, N. \tag{19}$$

The integrals for M (8) and for r (9) are trivial, and the final answers are shown in Table I for increasing orders of approximation. Also shown in this table for

comparison are the results of Gaussian quadrature using the weights and points for the integral [2].

$$\int_0^1 dssf(s). \tag{20}$$

TABLE I

SUCCESSIVE APPROXIMATIONS TO THE INTEGRAL I_1

N	Variational approximation	Gaussian approximation
1	0.1851852	0.2142857
2	0.1851852	0.1840796
3	0.1861952	0.1863572
4	0.1861952	0.1861892
5	0.1862006	0.1862015
6	0.1862006	0.1862006
exact	$2 - \pi/\sqrt{3} = 0.18620064$	

We observe that both methods work extremely well, there being nothing in Table I to prove superiority of either method.

Example 2.

$$I_2 = \int_0^\infty dx \int_0^\infty dy 2/(x + y + 1)^3. \tag{21}$$

We set

$$W = (x + y + 1)^3/2 \tag{22}$$

and now must decide what basis of functions to use to expand $1/W$. Our first try is the following

$$u_{nm} = \frac{1/a}{(1 + x/a)^m} \frac{1/a}{(1 + y/a)^n}. \tag{23}$$

With this basis all the integrals factor into two one-dimensional integrals of the form

$$\int_0^\infty dx \frac{x^l}{(1 + x)^k} \tag{24}$$

which are easily tabulated. In accordance with the behavior of $1/W$ as x or y goes to infinity (and to insure convergence of the integrals) we start the indices m and n at the value 3 and then systematically increase the two-dimensional array of basis functions to get overall matrix sizes $N = 1, 4, 9, 16$, etc. The results, shown in Table II under the heading "first try", converge very poorly.

TABLE II

SUCCESSIVE APPROXIMATIONS TO THE INTEGRAL I_2

N	first try	second try
1	0.80843465	0.95552585
4	0.91096467	0.99899305
9	0.94608335	0.99998307
16	0.96320503	0.99999976
25	0.97320695	0.99999999
36	0.98031977	
49	0.98144121	

The reason for this poor result may be found in a careful study of the asymptotic behavior of $1/W$. If we introduce polar variables

$$\begin{aligned} x &= R\cos\theta \qquad 0 \leqslant \theta \leqslant \pi/2 \\ y &= R\sin\theta \qquad 0 \leqslant R < \infty, \end{aligned} \tag{25}$$

then we see that as R goes to infinity the function $1/W$ goes as R^{-3} while the expansion functions (23) go as R^{-6}. Actually one can show that the expansion coefficients in this case must decay as

$$(C_N)^2 \xrightarrow[N\to\infty]{} O(N^{-2}) \tag{26}$$

and this does explain the slow convergence seen in Table II.

As a remedy we shall repeat the calculation using the following basis:

$$u_{nm} = \frac{1/a^2}{(1 + R/a)^{n+m}} \times \begin{cases} \sin^m\theta & m \geqslant 0 \\ \text{or} & \\ \sin^{m-1}\theta\cos\theta & m \geqslant 1 \end{cases}$$

where

$$n \geqslant 3.$$

All the required integrals are again easy; the results are shown in Table II under the heading "second try" and we see an extremely rapid convergence. This example emphasizes the importance of choosing appropriate basis functions, but exactly how to do this in each problem is something the analyst will have to discover for himself.

Example 3.

$$I_3 = \int_0^1 ds \int_0^1 dtst(1 - s)/[1 - t + ts(1 - s)]^2. \tag{28}$$

This integral arises in calculating the fourth order self-energy term for spinless particles associated with the Feynman diagram having two overlapping bubbles when we set the external 4-momentum equal to zero and all the internal masses equal to one.

First we apply the Gauss quadrature prescription [2] for the product of the two one-dimensional integrals

$$\int_0^1 s\, ds \int_0^1 t\, dtf(s, t), \tag{29}$$

and the results, shown under column "Gauss 1" in Table III, are seen to converge very poorly.

TABLE III

SUCCESSIVE APPROXIMATIONS TO THE INTEGRAL I_3

N	Gauss 1	Gauss 2	Variational
1	0.3594	0.67949	0.70880010
4	0.5885	0.74665	0.77732984
9	0.6795	0.77031	0.78107968
16	0.7189	0.77735	0.78128913
25	0.7389	0.77961	0.78130121
36	0.7505	0.78045	0.78130228
49	0.7579	0.78083	0.78130239
64	0.7629	0.78101	

The reason for this poor result lies in the fact that the denominator in (28) vanishes and makes the integrand singular at the two corners of the square:

$$t = 1, \quad s = 0 \qquad \text{and} \qquad t = 1, \quad s = 1. \tag{30}$$

One standard remedy is to subtract off the singular part; and in the column "Gauss 2" of Table III we show the results of the same Gauss quadrature applied to the integral I_3 after adding and subtracting

$$\int_0^1 ds \int_0^1 dtst(1-s)\left[\frac{1}{(1-t+s)^2}+\frac{1}{(2-t-s)^2}\right] = \tfrac{1}{3}(4\ln 2 - 1). \quad (31)$$

These results are an improvement, but still not terribly good; to continue the process of subtracting off the singular parts seems a cumbersome program.

Now we will try our variational method for I_3. We take

$$W = [1 - t + ts(1-s)]^2$$

and ask, What is the most important feature that we want to build into the expansion functions? The answer is the singularities at the points (30) which are represented by the terms in (31) above. We can simplify by noting that the integrand is symmetric about $s = 1/2$, so we just integrate s from 0 to 1/2 and multiply the result by 2. We have now only the first singularity to worry about, and we choose for our basis

$$u_{nm} = \frac{2^n s^{n-1}(1-t)^{n-1}}{(1-t+s)^2} \qquad n, m \geqslant 1. \quad (32)$$

In order to do the integrals the following procedure is used:

$$\int_0^{1/2} ds \int_0^1 dt = \int_0^{1/2} ds \int_0^{2s} dt + \int_0^1 dt \int_0^{t/2} ds \quad (33)$$

then introduce new variables $t = 2sx$ in the first term and $s = ty/2$ in the second. All the integrals then factor into products of one dimensional integrals which are straightforward to evaluate. (It must be admitted that rather a longwinded mess of algebra is involved here.) The final results are shown in the last column of Table III and we see extremely good convergence: We gain a factor of ten in accuracy at each step. (This calculation took six seconds on a fast computer.)

Generalizations of the Variational Method

Our variational principle was for integrands of the special form $1/W$; now consider the integral

$$\int \frac{1}{W_1 W_2 W_3 \cdots W_k} \quad (34)$$

where we would like to handle each W_i separately. We can construct the following variational expression

$$J = \int \chi^{(1)} + \int \phi^{(k)} + \sum_{i=2}^{k} \int \chi^{(i)}\phi^{(i-1)} - \sum_{i=1}^{k} \int \chi^{(i)} W_i \phi^{(i)} \tag{35}$$

which depends on two sets of trial functions $\phi^{(i)}$ and $\chi^{(i)}$. If we vary the χ's we get equations for the ϕ's which are trivially solved to tell us that the exact solutions are

$$\phi^{(i)} = \frac{1}{W_1 W_2 \cdots W_i}. \tag{36}$$

And conversely varying the ϕ's gives us equations for the χ's which lead to the exact solutions

$$\chi^{(i)} = \frac{1}{W_i W_{i+1} \cdots W_k} \tag{37}$$

and then the stationary value of (35) is just the integral (34). If we now make linear expansions of the trial functions $\chi^{(i)}$ and $\phi^{(i)}$ (each can have a different set of basis functions) we come to a result in which the integral (34) is given by a generalization of (13) as follows:

$$r \cdot M_k^{-1} \cdot N_k \cdot M_{k-1}^{-1} \cdot N_{k-1} \cdot \cdots N_2 \cdot M_1^{-1} \cdot p \tag{38}$$

where M_i is the matrix of W_i between the functions $\chi^{(i)}$ and $\phi^{(i)}$, and N_i is the matrix of overlap integrals between $\chi^{(i)}$ and $\phi^{(i-1)}$. Without going into more detail we will just report that we have used this technique on the integral I_3, Eq. (28), where we took

$$W_1 = W_2 = [1 - t + ts(1 - s)]; \tag{39}$$

the results were just as good as those shown for the original variational results in Table III, and the labor involved was somewhat less.

Now let us just briefly mention an even greater generalization of this variational method [3]. Start again by focusing on some simple expression $W(x)$ but consider the general integral

$$\int F(W) \tag{40}$$

for an arbitrary function F. Imagine that we take some complete (and for simplicity orthonormal) set of functions $u_n(x)$. Then we can have $W(x)$ represented by its matrix elements

$$W_{mn} = \int u_m W u_n . \tag{41}$$

If we assume that $u_0 = 1$ (which can be arranged by appropriate choice of the volume element), then we see

$$\int W = W_{00}\,; \tag{42}$$

$$\int W^2 = \sum_n W_{0n} W_{n0}\,; \tag{43}$$

$$\int W^3 = \sum_{nm} W_{0n} W_{nm} W_{m0} \tag{44}$$

etc.

where we have used the completeness property

$$\sum_n u_n(x)\, u_n(x') = \delta(x - x'). \tag{45}$$

Now we take the big step and say: To evaluate the integral (40) build the matrix $\langle W \rangle$ whose elements are given by (41), compute the matrix

$$\langle F \rangle = F(\langle W \rangle) \tag{46}$$

and take its 0–0 element for the answer. The approximation we make is to use a truncated (finite dimensional) matrix for $\langle W \rangle$, and the successive steps of approximation amount to increasing the size of the basis kept. In order to evaluate (46) in general one can always transform $\langle W \rangle$ to diagonal form, put in the function F of its eigenvalues, and then transform back to the original representation. We have not tried any examples of this general method, but it should be worth further study.

References

1. See, for example, R. W. Hamming, "Numerical Methods for Scientists and Engineers," Section 10.7. McGraw-Hill, New York, 1962.
2. M. Abromowitz and I. A. Stegun, "Handbook of Mathematical Functions," page 921. Dover Publications, New York, 1965.
3. The following method was inspired by the work of D. O. Harris, G. G. Engerholm, and W. D. Gwinn, *J. Chem. Phys.* **43**, 1515 (1965).