13.0 Effective Use of the Quadrature Software

A. Introduction

The quadrature software in MATH77 is designed to be efficient and reliable even if the user does nothing special. For most one dimensional problems, one will get quite satisfactory results without taking any special care, even for most of the special cases discussed below. But if function values are expensive or one is computing a large number of related integrals, and particularly in the case of multi–dimensional integrals, one can obtain benefits in accuracy, efficiency, and/or reliability by making use of the ideas discussed below.

The sections which follow consider the following.

B. Analytic Integration

One should not overlook the possibility of using a computer algebra system to obtain an integral, part of a multiple integral, or even part of a single integral in order to obtain a better behaved function for the numerical integration.

Frequently an integral can be reduced to a special function such as those in Chapter 2 of MATH77. The routines for computing these functions should be both more reliable and more efficient than doing the integration numerically.

C. Estimating Noise Levels

Options 4 and 5 in the quadrature routines allow one to provide an estimate of the absolute and relative errors in computing the function, respectively. The quadrature routines attempt to make an estimate of these errors if no data are provided by the user, but it is very difficult to tell the difference between a noisy function, and a function which just needs to be sampled on a finer mesh. If you know of cancellation errors, or if the function values are obtained from another computation for which error estimates are available, or if part of the function is computed using a table lookup which is known to have errors of a certain level, you will reduce the risk of the quadrature routine working much harder than necessary if you provide this information. Note than the multiple quadrature routine works by applying the one dimensional routine to the results of applying the one dimensional routine to an inner integral which in turn may be the result of applying the one dimensional routine to yet another inner integral, etc. In this case the routines know of the error estimates from the interior quadrature and make use of these estimates in estimating the value of these parameters for the outer integrations.

D. Multi–dimensional Quadrature

The cost of computing typically goes up very rapidly with the dimension. The routines that we provide are meant to be used primarily for one, two, and three dimensional integrals. They may be appropriate for some higher dimensional problems, particularly if one has an irregular boundary, or outer integrals are functions of inner integrals. Effective integration of high dimensional integrals requires scattering the points in a way that is not possible with the approach used in the MATH77 routines. Most commonly such problems are attacked using Monte Carlo methods, preferably with serious thought given to methods for reducing the variance. For regular regions, the methods in [1] and [2] are likely to be a good choice when they apply. Also see the very nice review article by Spanier and Maize [3], and the recent book by Sloan and Joe [4].

When using the routines in MATH77 don't forget that singularities may be introduced by the form of the boundary, and that all singularities are best removed if at all possible.

E. Dealing with Singularities

The methods used in the MATH77 routines are based on approximating the function by a polynomial interpolating the function at judiciously chosen points. Unfortunately polynomials do not do a good job of approximating certain functions. If the function has an infinite low order derivative some place near the interval of integration (including off the real line in the complex plane), taking some action to remove (or weaken) the singularity can make a big difference in performance. Thus, let $f(x)$, the function being integrated, have the form $f(x) = u(x)s(x)$, where u is the unsmooth part, and s is the smooth part. Some examples for u(x) are $(x-a)^\alpha$, $(x^2-a^2)^\alpha, \log(x-a)$, and $1/(x^2+a^2)$, where α is not an integer, and the singularity is at a in all but the last case where the singularity is at $\pm ia$ and a is presumably small relative to the length of the interval.

It may not always be clear how to split functions. For example, given a factor of $\sqrt{x^2-a^2}$ one might set $u(x)$ to this factor, or one might set $u(x)=\sqrt{x-a}$ and let $s(x)$ contain the factor $\sqrt{x+a}$ (assuming x and a are both positive).

When there are singularities in the middle of the range of integration, even if one does nothing else, one is better off to break the interval in two pieces so all singularities occur at the endpoints of the interval of integration. If there are singularities at both endpoints, it is best in most cases to break the interval in the middle, so that all one is ever dealing with in a single numerical integration is a function with a singularity at a single end point. If you have something like a factor of $1/\sqrt{p(x)}$, where p is a polynomial, take the trouble of finding the roots of p and break up the interval of integration so that there are no internal singularities.

The first of the three approaches we consider takes advantage of the fact that the unsmooth part of a function frequently can be integrated analytically. Following Krylov [5, p.203]

$$f(x)=f_1(x)+f_2(x), \text{ where}$$
$$f_1(x)=u(x)\sum_{j=0}^{k-1}\frac{s^{(j)}(a)}{j!}(x-a)^j$$
$$f_2(x)=u(x)\left[s(x)-\sum_{j=0}^{k-1}\frac{s^{(j)}(a)}{j!}(x-a)^j\right].$$

Assuming the required derivatives of s can be computed and that the integral of f_1 can be computed analytically, one has the simpler problem of integrating f_2. The singularity has been weakened by increasing the order of the first infinite derivative by k. This can make a significant difference in performance.

Lether [6] discussed this approach in more detail for the case when the singularity is not on the real axis.

The second approach is to make a change in variable that weakens the singularity. This approach has the advantage that when it works it can remove the singularity entirely. It has the disadvantage that the appropriate transformation may be difficult to find, such a transformation may not exist, and when one is some distance from the singularity, one may be better off without the transformation.

Consider

$$\int_a^b (x-a)^\alpha s(x)\,dx.$$

With $\xi=(x-a)^{1/\beta}$, $(x=a+\xi^\beta)$ this is transformed to

$$\int_0^{(b-a)^{1/\beta}} \xi^{\beta(\alpha+1)-1}s(\beta\xi^{\beta-1}+a)\,d\xi.$$

In order to get a "nice" integral, we would like to have both $\beta(\alpha+1)-1$, and $\beta-1$ be small positive integers. $\beta=2$ satisfies these conditions for both $\alpha=-1/2$ and for $\alpha=1/2$. The one dimensional subroutines in MATH77 make this kind of transformation (once or twice) when they think they have determined there is a singularity at a. Note that $\beta=2$ weakens all singularities at a. But a better choice when $\alpha=k/3$ (k a small integer ≥ -2) is $\beta=3$, which you will have to do yourself if you want it.

The third approach is not to use the MATH77 routines, but to develop your own quadrature formula (and routine) using $u(x)$ as a weight function as discussed in "Special Weight Functions" below.

F. Iterated Integrals

Since

$$\int_a^b\int_a^x\cdots\int_a^x f(x)(dx)^{k+1}=\int_a^b\frac{(b-x)^k}{k!}f(x)dx,$$

one should never treat the left hand side as a multiple integral when one can just as easily integrate the right hand side as a one–dimensional integral. (One can get this result using repeated integration by parts.)

G. Infinite Range

Consider (one can always translate the integrations variable to start at 0)

$$\int_0^\infty f(x)\,dx$$

and assume there is a monotone strictly decreasing function $\varphi(x)$ which decreases with a rate somewhat like that for $|f|$, preferably providing some reasonable approximation to an upper bound for $|f(x)|$ for large x. Once again we offer three approaches.

From ones knowledge of φ, or by sampling $f(x)$ for large x, determine a value for X such that

$$\left|\int_0^X f(x)\,dx-\int_0^\infty f(x)\,dx\right|<.5\times\ \text{(error required)}.$$

Then use the finite integral as an approximation for the infinite integral, asking for enough additional accuracy in integrating it to compensate for the reduction in range. If one uses this approach one should not pick X so large that f has underflowed to 0. The one–dimensional routines make checks for discontinuities, both for enhanced reliability, and to encourage users to provide functions which are smooth, which greatly improves the efficiency of the integration. If f has underflowed, f appears to be a flat 0 for a part of the interval, with an infinite relative jump at some point to a nonzero value. Locating the point of this discontinuity is time consuming and the resulting diagnostic is liable to be confusing to someone even if it isn't to you. Since the integration of this kind of problem will typically require a wide range in the mesh, the integration will probably not be as efficient as one might hope for.

The second approach involves making a change of variable. Assume that we have selected $\varphi(x)$ so that $\varphi(\infty) = 0$, and the inverse function is known and differentiable. Let $\xi = \varphi(x)$ and we have

$$\int_0^\infty f(x)\,dx = \int_0^{\varphi(0)} -\frac{d\varphi^{-1}(\xi)}{d\xi} f(\varphi^{-1}(\xi))\,d\xi.$$

Examples of different φ's are given in the table below. We assume that by a crude approximation over a wide range of x, that any required values of α and β have been estimated.

$\boldsymbol{\varphi(x)}$	$\boldsymbol{\varphi(0)}$	$\boldsymbol{-\frac{d\varphi^{-1}(\xi)}{d\xi}}$	$\boldsymbol{\varphi^{-1}(\xi)}$
$\frac{\alpha}{1+\beta * x^2}$	α/β	$\frac{\alpha\beta^{3/2}}{2\xi^{3/2}\sqrt{\alpha-\xi}}$	$\sqrt{\frac{\alpha-\xi}{\beta\xi}}$
$e^{-\alpha(x-\beta)}$	$e^{\alpha\beta}$	$1/\alpha\xi$	$\frac{-\log(\xi)}{\alpha}+\beta$
$e^{-\alpha(x-\beta)^2}$	$e^{-\alpha\beta^2}$	$\frac{1}{2\alpha\xi}\sqrt{\frac{-\alpha}{\log\xi}}$	$\sqrt{-\log(\xi)/\alpha}+\beta$

The hope is that $f(\varphi^{-1}(\xi))$ will cancel the part of the denominator that is going to 0 as ξ approached 0. This cancellation can be done analytically if possible, otherwise it may be best to fudge the 0 to a slightly larger number. It should also be noted that these transformations may be useful anytime the limits on the original integral are widely separated. If these limits are a and b, then in the transformed integral the limits are $\phi(b)$ and $\phi(a)$.

There are two problems suggested by the above table. First, if one can not do some cancellations analytically, there may be problems with underflow in the denominator. Second, the transformation is introducing a singularity which one should probably deal with as is described in the section "Dealing with Singularities" above. Finally, we should note that we have essentially no experience using this approach and would appreciate hearing of your experience if you should try it.

The third approach, is to use a weight function as described below. This approach can not be used with the MATH77 software.

H. Special Weight Functions

Here we are concerned with the integration of functions of the form

$$\int_a^b w(x)f(x)\,dx,$$

where w(x) is called the weight function, and f(x) is presumably a fairly well behaved function that it is reasonable to approximate with a polynomial. In some of the cases listed below, one could choose to integrate part of the interval using special formulas designed to cope with the singularity in w, and integrate the rest of the interval using the one dimensional routines provided here.

In [7] we find the following cases listed

Name	**w(x)**	**Interval**
Moments	x^k	$(0,1)$
	$\sqrt{b-y}$	(a,b)
	$1/\sqrt{b-y}$	(a,b)
	$1/\sqrt{1-x^2}$	$(-1,1)$
	$1/\sqrt{(x-a)(b-x)}$	(a,b)
	$\sqrt{1-x^2}$	$(-1,1)$
	$\sqrt{(x-a)(b-x)}$	(a,b)
	$\sqrt{x/(1-x)}$	$(-1,1)$
	$\sqrt{(x-a)/(b-x)}$	(a,b)
	$\log x$	$(0,1)$
Laguerre	e^{-x}	$(0,\infty)$
Hermite	e^{-x^2}	$(-\infty,\infty)$
Filon	$\cos\omega x$	(a,b)
Filon	$\sin\omega x$	(a,b)

If you would like to derive your own formulas, particularly if you would like formulas with a built-in error estimate, we recommend the algorithm of Patterson [8].

I. Indefinite Integrals

The quadrature routines in MATH77 are not designed to be useful for indefinite integration. Instead of solving

$$\int_a^t f(t)\,dt,$$

one can solve the differential equation

$$y' = f(t), \quad y(a) = 0.$$

If one of the routines in Chapter 14.1 is used for this purpose, one should skip the evaluation of $f(t)$ when the corrected derivative is being computed. This approach can also be useful for a definite integral when $\mathbf{f}(t)$ is a vector valued function and computations for some of the components can be reused in others.

When solving Volterra integral equations, if one can weaken singularities in f sufficiently (perhaps using other techniques in this chapter), so that using a uniform mesh is appropriate, we believe formulas based on using the trapezoidal rule with difference corrections are a reasonable choice. See [9, pp. 155–156] for the discussion on Gregory's formula and the Gauss summation formula. Probably the easiest way to derive the appropriate formulas near the end of the interval is to think in terms of using the Gauss summation formula for all points, but using polynomial extrapolation to obtain the differences that would otherwise require using a function value outside the interval. (We find it most convenient to think of the mean central differences as the average of backward differences at two other points and to use the fact that $\nabla^k f_n = \nabla^k f_{n+1} - \nabla^{k+1} f_{n+1}$ to get values for the differences near the left endpoint, and to use $\nabla^k f_{n+1} = \nabla^k f_{n+1} - \nabla^k f_n$ near the right endpoint.) The difference between the result at two interior points can be expressed in terms of the difference between mean central differences at two different points, giving a bandwidth of $k+3$ if the last difference used is the k^{th} mean central difference, $\mu\delta^k f$.

J. Cauchy Principal Values

Suppose f has a single singularity at $x = \xi$ in the interval $[a, b]$, and that although the integrals

$$\int_a^{\xi} f(x)\,dx, \text{ and } \int_{\xi}^{b} f(x)\,dx$$

don't exist, cancellation is such that the limit

$$\lim_{\varepsilon \to 0} \Bigl(\int_a^{\xi-\varepsilon} f(x)\,dx + \int_{\xi+\varepsilon}^{b} f(x)\,dx \Bigr)$$

does exist. This limit is called the Cauchy principal value of the integral. If you can, use the first approach in Section E for dealing with singularities, so that the Cauchy principal value does not need to be computed numerically. (Keep in mind that the problems with cancellation error mentioned below will still be present.) Else, we propose the following (untried) method for solving such problems.

First determine ξ as accurately as possible, i.e. down to the last bit. The zero finding program DZERO in Chapter 8.1 applied to $1/f$ could be used for this purpose. Assuming ξ is closer to a than to b (with obvious modifications in the opposite case), compute

$$I_1 = \int_0^{a-\xi} \left[f(\xi + x) + f(\xi - x) \right] dx,$$

using DINT1, the double precision one–dimensional quadrature program. If it is convenient, compute the sum in such a way as to minimize the cancellation that arises in summing the f values. Sometimes this might be done analytically, sometimes one might be able to do the calculation of the f's near ξ in an extended precision. One should also let DINT1 know how large the absolute error in the integrand can be, since when f gets large there is going to be more cancellation than DINT1 would expect from the value of the difference. Because of the problems with cancellation error, it is probably best to allocate most of the allowable error to computing I_1.

Then compute

$$I_2 = \int_{2\xi-a}^{b} f(x)\,dx,$$

using DINT1, with option 11 to indicate there is a singularity at $x = \xi$. If the singularity is close to a, one should probably use a negative value for the K11 associated with this option.

The final result is of course given by $I_1 + I_2$.

K. Undefined Integrals

We don't have much to say here except that when dealing with extremely complicated expressions, it is quite possible to end up defining a problem for which the integral does not exist. If you should do this you may get a diagnostic telling you that this is the case, but then again you may not. It is not easy to tell the difference between an integrand with a narrow very high peak, and one that goes off to infinity. But if you don't get the diagnostic you should observe that the integral seems to be very hard to compute, and the accuracy is terrible. When this happens to you at least consider the possibility that you have defined a problem whose best solution is "define a different problem." You may also get the diagnostic that the integrand is not integrable when in fact it is, however your first inclination should be to trust the diagnostic.

References

1. A. H. Stroud, **Approximate Calculation of Multiple Integrals**, Prentice-Hall, Englewood Cliffs, N. J. (1971).
2. Ronald Cools and Philip Rabinowitz, *Monomial cubature rules since "Stroud": a compilation*, **J. Comp. and Applied Math. 48** (1993) 309–326.
3. Jerome Spanier and Earl H. Maize, *Quasi-random methods for estimating integrals using relatively small samples*, **SIAM Review 36**, 1 (March 1994) 18–44.
4. I. H. Sloan and S. Joe, **Lattice Methods for Multiple Integration**, Oxford Univ. Press, Oxford (1995).
5. Vladimir Ivanovich Krylov, **Approximate Calculation of Integrals**, Macmillan, New York (1962) 357 pages. Translated by Stroud.

6. F. G. Lether, *Subtracting out complex singularities in numerical integration*, **Math. of Comp. 31** (1977) 223–229.

7. Milton Abramowitz and Irene A. Stegun, **Handbook of Mathematical Functions**, *Applied Mathematics Series 55*, National Bureau of Standards (1966) Chapter 25, 888–891.

8. T. N. L. Patterson, *Algorithm 672: Generation of interpolatory quadrature rules of the highest degree of precision with preassigned nodes for general weight functions*, **ACM Trans. on Math. Software 15**, 2 (June 1989) 137–143.

9. F. B. Hildebrand, **Introduction to Numerical Analysis**, McGraw-Hill, New York (1956) 511 pages. A reprint of a later edition is available from Dover.

10. H. Brass and G. Hämmerlin, editors, **Numerical Integration IV, Proceedings of the Conference at the Mathematical Research Institute, Oberwolfach, Nov. 8–14, 1992**, *International Series of Numerical Mathematics 112*, Birkhäuser Verlag, Basel (1993).

Fred T. Krogh, JPL, August 1995. Material added by Krogh at Math à la Carte, August 2009.