5.8 Multivariable Integration

Multiple integrals are much more varied than single integrals, mainly because of the much greater variety of integration regions. These regions can be relatively simple, such as a rectangle, or more complicated, such as the surface of a torus. To deal with this variety, many specialized formulas and programs have been developed. In the limited space available here, we will survey a few of the more important formulas and ideas thaat are used in evaluating multiple integrals.

Consider the multiple integral

$$I(f)=\int_D f(x,y)dxdy \qquad (5.8.1)$$

where D is a region in the xy-plane. One of the simplest ideas used in evaluating such an integral is to write it as iterated simple integrals. Sometimes the definition of D leads to an easy formulation as iterated integrals,

$$I(f)=\int_a^b\int_{c(x)}^{d(x)} f(x,y)dy\ dx \qquad (5.8.2)$$

In other cases, a change of variables may be needed or may lead to a simpler formulation. For example, if the region has either angular or radial symmetry about the origin, then the use of polar coordinates is probably a good idea.

After obtaining an integral in the form (5.8.2), we can apply single variable integration formulas to each of the integrals in (5.8.2). This is simple to carry out, and it is often efficient and effective. The resulting formulas look like

$$\tilde{I}(f)=\sum_{i=1}^{n}\sum_{j=1}^{m} u_{in}v_{jm}f(x_{in},y_{jm}), \qquad (5.8.3)$$

and m may depend on i. These formulas are called *product formulas*, because the nodes $\{(x_i,y_j)\}$ are formed from the cross-product set of $\{x_i\}$ and $\{y_j\}$, giving a regular rectangular pattern. Following are illustrations of this procedure.

<u>Example</u> 1. Let D be a rectangle,

$$D=\{(x,y)\,|\,a\le x\le b,\ c\le y\le d\} \qquad (5.8.4)$$

Then use (5.8.2) with constant c and d. Apply n and m point Gauss-Legendre quadrature to each integral in (5.8.2), leading to (5.8.3). This is a quick and often very satisfactory way of evaluating (5.8.2). In contrast, see Lyness (1983) for a discussion of the dangers of using iterated automatic single variable integration programs.

2. Let D be the ellipse

$$D=\{(x,y)\,|\ \frac{x^2}{a^2}+\frac{y^2}{b^2}\le 1\} \qquad (5.8.5)$$

Use the change of variables

$$x=ar\cdot\cos\theta, \qquad y=br\cdot\sin\theta$$

Then (5.8.1) becomes

$$I=ab\int_0^1\int_0^{2\pi} rf(ar\cdot\cos\theta,\ br\cdot\sin\theta)\,d\theta\, dr \qquad (5.8.6)$$

Because the integrand is periodic in θ, use the trapezoidal rule to approximate the integral with respect to θ. For the integration in r, we could use Gauss-Legendre quadrature. However, if many such integrals are to be evaluated, it is more efficient to use a Gauss quadrature formula with weight function $w(r)=r$:

$$\int_0^1 rF(rdr) \doteq \sum_{j=1}^{n} w_j F(r_j) \qquad (5.8.7)$$

Tables for this are given in Stroud-Secrest (1966).

For integrals that have a singularity of radial type at the origin, the above often results in a more manageable problem. For example,

$$\int_D \frac{q(x,y)}{\sqrt{x^2+y^2}} dxdy$$
$$= ab\int_0^1\int_0^{2\pi} g(ar\cdot\cos\theta,\ br\cdot\sin\theta)[a^2\cos^2\theta+b^2\sin^2\theta]^{-1/2} d\theta dr \qquad (5.8.8)$$

If g(x,y) is a well-behaved differentiable function, then the right-hand integral has a smooth integrand.

3. Later in this section, we will be considering integrals over triangles, and a central role will be played by

$$I=\int_0^1\int_0^{1-s} g(s,t)dt\ ds \qquad (5.8.9)$$

Here the integration region D is the triangle with vertices (0,0), (0,1), and (1,0). There are many formulas for evaluating (5.8.9), as will be discussed later. An important special case of such integrals I is

$$I = \int_0^1\int_0^{1-s} \frac{h(s,t)}{(s^2+t^2)^\alpha} \qquad (5.8.10$$

with $\alpha<1$ and h(s,t) a continuously differentiable function. One approach to evaluating (5.8.10) is to use extrapolation formulas based on asymptotic error formulas for common quadrature methods applied to the integral; see Lyness (1976). We will give another approach, taken from Duffy (1982), which uses a carefully chosen change of variables.

In (5.8.10), let

$$s=(1-y)x, \quad t=yx, \qquad 0\le x,y\le 1 \tag{5.8.11}$$

Then (5.8.10) becomes

$$I = \int_0^1 \frac{1}{[(1-y)^2+y^2]^\alpha} \int_0^1 x^{1-2\alpha} h((1-y)x,yx)\,dx\,dy \tag{5.8.12}$$

The inner integral can be approximated by Gaussian quadrature with a weight function $w(x)=x^{1-2\alpha}$, and the outer integral can be evaluated with ordinary Gauss-Legendre quadrature. One of the more important cases of (5.8.10) is $\alpha=1/2$: the weight function $w(x)=1$, and both integrals in (5.8.12) can be approximated with Gauss-Legendre quadrature.

Integration over triangular regions Numerical integration over triangular regions is used in the approximate solution of partial differential equations and multivariable integral equations, and it is used in constructing numerical integration formulas for non-triangular regions. The topic is closely connected to interpolation over triangular regions, and we will be using some of the notation used earlier for such interpolation, in §3.8, following formula (3.8.15).

Let Δ be a triangle in the xy-plane with vertices $v_i=(x_i,y_i)$, $i=1,2,3$. Introduce the unit simplex

$$\sigma = \{(s,t)\,|\,0\le s,t,s+t\le 1\},$$

and give a parametric representation of Δ using

$$T(s,t) = uv_1+sv_2+tv_3, \quad (s,t)\in\sigma \tag{5.8.13}$$

with $u=1-s-t$. Then

$$\int_\Delta f(x,y)\,dx\,dy = 2A\int_\sigma f(T(s,t))\,ds\,dt \tag{5.8.14}$$

with A the area of Δ,

$$A = |a|, \quad a = \frac{1}{2}\det\begin{bmatrix} x_2 - x_1 & x_3 - x_1 \\ y_2 - y_1 & y_3 - y_1 \end{bmatrix}$$

formula (5.8.14) reduces the problem of integrating over an arbitrary region Δ to that of integrating an equally smooth function over the unit simplex σ.

We seek formulas

$$I_n(g) = \sum_{j=1}^{n} w_j g(q_j) \doteq I(g) = \int_\sigma g(s,t)\,ds\,dt \qquad (5.8.15)$$

with $q_j = (s_j, t_j) \in \sigma$. In some cases the nodes are already specified, and in other cases we can allow both the nodes and weights to be chosen freely. The central theme in choosing these parameters is to make the formula (5.8.15) exact for $g(s,t)$ an arbitrary polynomial of degree as large as possible. We say the formula (5.8.15) has degree of precision d if (1) $I_n(g) = I(g)$ for any polynomial $g(s,t)$ of degree $\leq d$, and (2) $I_n(g) \neq I(g)$ for some polynomial $g(s,t)$ of degree $d+1$.

A straightforward procedure for obtaining formulas of arbitrary degrees of precision is to integrate the interpolating polynomials developed in chapter 3 following (3.8.15). Integrating the linear interpolating polynomial $p_1(s,t)$ of (3.8.20),

$$\int_\sigma g(s,t)\,ds\,dt \doteq \frac{1}{6}[g(0,0) + g(0,1) + g(1,0)] \qquad (5.8.16)$$

Integrating the quadratic interpolating polynomial $p_2(s,t)$ of (3.8.25) yields

$$\int_\sigma g(s,t)\,ds\,dt \doteq \frac{1}{6}[g(\tfrac{1}{2},\tfrac{1}{2}) + g(\tfrac{1}{2},0) + g(0,\tfrac{1}{2})] \qquad (5.8.17)$$

The degrees of precision of these formulas are 1 and 2, respectively. Formulas with a higher degree of precision are obtained by integrating higher degree interpolation formulas.

To obtain some idea of the connection between the degree of precision and the number of node points, consider the degrees of freedom in the formula and the constraints imposed by the degree of precision. If no conditions are placed on the nodes and weights, other than that the nodes lie in σ, then there are 3n degrees of freedom in determining (5.8.15). To integrate exactly all polynomials of degree$\le$d, it is necessary and sufficient to numerically integrate exactly the monomials

$$g(s,t)=s^i t^j, \qquad i+j\le d, \quad i,j\ge 0. \tag{5.8.18}$$

There are (d+1)(d+2)/2 such monomials, and for $I_n(g)$ to integrate them exactly will impose (d+1)(d+2)/2 constraints on the formula (5.8.15). If we require the number of degrees of freedom to bound the number of constraints imposed by the degree of precision being d, then we would expect to require that

$$n\ge\frac{(d+2)(d+1)}{6} \tag{5.8.19}$$

The author does not know whether this condition is actually necessary; but all of the formulas $I_n(g)$ that are given in Stroud (1971, pp. 306-315) and Lyness-Jesperson (1975) satisfy it, in some cases with equality. For a more rigorous lower bound for n, see Stroud (1971, p. 118).

<u>Examples</u> We give three efficient integration formulas over σ.

1. The formula

$$\int_\sigma g(x,t)ds\ dt \doteq \tfrac{1}{2}g(\tfrac{1}{3},\tfrac{1}{3}) \tag{5.8.20}$$

has degree of precision 1. It is sometimes called the *centroid rule*, since $(\frac{1}{3},\frac{1}{3})$ is the centroid of σ. It can be considered to be a two-dimensional generalization of the midpoint rule.

2. The 4 point formula

$$\int_\sigma g(s,t)ds\,dt \doteq -\frac{9}{32}f(\frac{1}{3},\frac{1}{3}) + \frac{25}{96}[f(\frac{1}{5},\frac{1}{5})+f(\frac{1}{5},\frac{3}{5})+f(\frac{3}{5},\frac{1}{5})] \tag{5.8.21}$$

has degree of precision 3. Note that one of the weights is negative, a generally undesirable property.

3. The 7 point formula

$$\int_\sigma g(s,t)ds\,dt \doteq \frac{9}{40}g(\frac{1}{3},\frac{1}{3})+\frac{1}{40}[g(0,0)+g(0,1)+g(1,0)] + \frac{1}{15}[g(0,\frac{1}{2})+g(\frac{1}{2},0)+g(\frac{1}{2},\frac{1}{2})] \tag{5.8.22}$$

has degree of precision 3. Although it uses more points than (5.8.21), it will have an advantage over (5.8.21) in practical computations, described below.

Most applications of the above formulas are to larger regions D which are decomposed into small triangular subregions. Thus D is the union of distinct triangles $\Delta_1,\ldots,\Delta_m$. To obtain convergence, we let $m\to\infty$ and

$$h_m = \underset{1\le i\le m}{\text{Maximum}}\left[\underset{p,q\in\Delta_i}{\text{Maximum}}\ |p-q|\right] \to 0 \tag{5.8.23}$$

Such a decomposition for a rectangular region is shown in Figure 5.5.

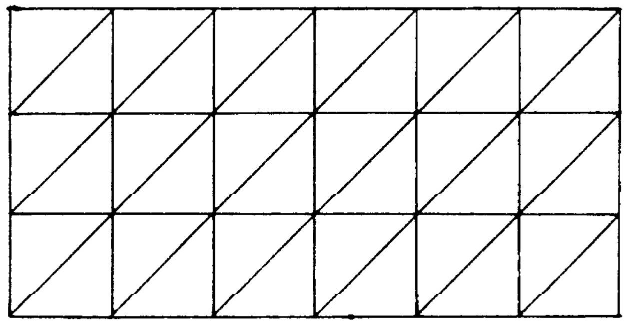

Figure 5.5 Triangular decomposition of a rectangle

If the integration formula $I_n(g)$ of (5.8.15) uses nodes that are strictly interior to σ, then the resultant formula for D will use mn nodes. This is the case with formulas (5.8.20) and (5.8.21). If however the formula (5.8.15) contains nodes on the boundary of σ, then such nodes will be shared with adjacent triangles and thus the number of integrand evaluations in D can be lessoned. To obtain a more precise calculation, consider triangular decompositions such as in Figure 5.5. To be specific, use the formula (5.8.22) over each triangle. Each vertex is shared among six triangles, and each midpoint of a side occurs in two triangles. Using this, we can show that the total number of integrand evaluations for the m triangles will be about 3m. For comparison, the formula (5.8.21) requires 4m evaluations, so that it is less efficient than using (5.8.22).

For the error in the formulas (5.8.15) for quadrature over σ, it can be shown that if $I_n(f)$ has degree of precision d, then

$$|I(g)-I_n(g)| \le c\cdot \underset{i+j=d+1}{\text{Maximum}} \left[\underset{(s,t)\in\sigma}{\text{Maximum}} \left| \frac{\partial^{d+1} g(s,t)}{\partial s^i \partial t^j} \right| \right] \qquad (5.8.24)$$

The proof uses Taylors theorem for functions of 2 variables, and it parallels the proof of the interpolation error result (3.8.26) in chapter 3. The constant c depends on the integration method, but it is independent of g. If this formula (5.8.24) is applied to the type of integration rule described in the preceding paragraph, then the replacement of $f(s,t)$ by $f(T(s,t))$, as indicated in (5.8.14), will lead to an error formula

$$\int_D f(x,y)dx\,dy - \sum_{j=1}^{m} \frac{1}{2}\text{Area}(\Delta_j) \sum_{i=1}^{n} w_i f(T_j(q_i)) = O(h_m^{d+1}) \qquad (5.8.25)$$

Thus the use of (5.8.22) will lead to an integration rule whose error is of order h_m^4.

The subject of multivariate quadrature is still relatively undeveloped, although a great deal has been written about it. An excellent general reference is Stroud (1970), as it contains both general theory and many special formulas. Other useful general references are Engels (1980) and Davis-Rabinowitz (1984, Chap. 5). For some additional formulas for triangular regions, see Lyness-Jespersen (1975). As an example of the different approaches to developing quadrature formulas for less standard regions, see Atkinson (1982) for formulas on the surface of a sphere and related regions.