Gibbs : Computational Physics

Chapter 1

Integration

The subject of integration is very old. The ancient Egyptians knew of the basic techniques of quadrature and applied them to calculate the areas of polygonal fields and the volumes of solids. Our starting point will be the same as that first presented by Bonaventura Cavalieri in 1635. As is very common in numerical techniques, we assume that the function that we wish to integrate can be represented in a sufficiently accurate manner by its value at a series of points, or nodes. The present problem is that of obtaining the best approximation to the integral of the function with the minimal number of nodes. Whether or not the nodes are evenly spaced in the independent variable will depend on the circumstances. For certain problems the function can be calculated conveniently only at equally spaced intervals (for example when it is the result of the solution of a differential equation). If the integrand can be evaluated at arbitrary values of the independent variable with no greater difficulty then, for a given accuracy, the integral can be calculated with fewer evaluations. For this reason we treat the case of equal and unequal intervals in parallel until we reach the subject of Gaussian integration which *requires* unequal spacing.

1.1 Classical Quadrature

Considering the diagram shown in Figure 1.1 we see that an estimate for the integral can be obtained by using the (linear) dotted lines as an approximation to the curve. Thus the integral can be represented by the sum of areas of a number of trapezoids, each with the form

$$\frac{1}{2}\left[f\left(x_i\right)+f\left(x_{i+1}\right)\right]\left(x_{i+1}-x_i\right). \tag{1.1}$$

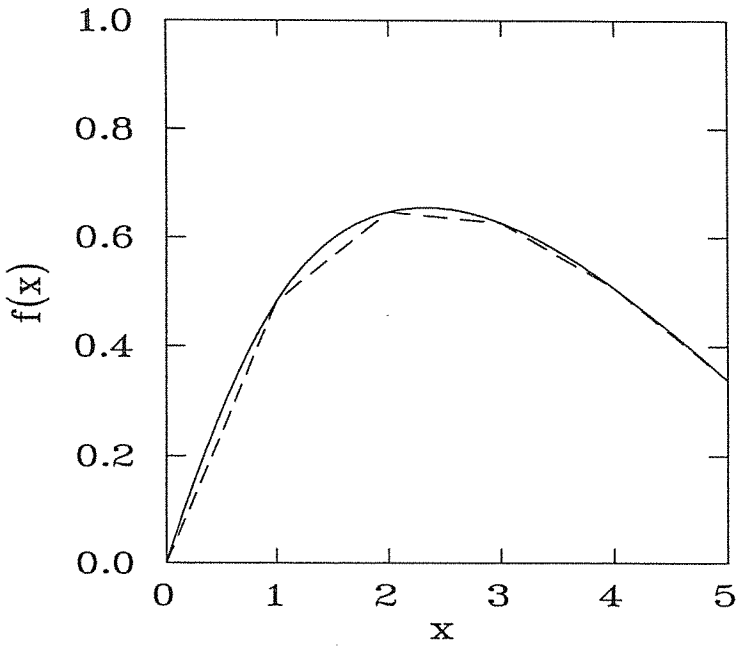

Figure 1.1: Representation of the Integrand by Straight-line Segments

Hence the integral is given approximately by:

$$\int_{x_1}^{x_n} f(x)dx \approx \frac{1}{2}\sum_{i=1}^{n-1}\left[f\left(x_i\right)+f\left(x_{i+1}\right)\right]\left(x_{i+1}-x_i\right) \tag{1.2}$$

$$\approx \frac{1}{2}\left(x_2-x_1\right)f_1+\frac{1}{2}\sum_{i=2}^{n-1}\left(x_{i+1}-x_{i-1}\right)f_i+\frac{1}{2}\left(x_n-x_{n-1}\right)f_n \tag{1.3}$$

or, more generally,

$$\int_{x_1}^{x_n} f(x)dx \approx \sum_{i=1}^{n} A_i f_i \tag{1.4}$$

where $f_i \equiv f(x_i)$

Arbitrary spacing		Equal spacing	
A_1	$= \frac{1}{2}(x_2 - x_1)$	A_1	$= \frac{1}{2}h$
A_2	$= \frac{1}{2}(x_3 - x_1)$	A_2	$= h$
A_3	$= \frac{1}{2}(x_4 - x_2)$	A_3	$= h$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
A_{n-2}	$= \frac{1}{2}(x_{n-1} - x_{n-3})$	A_{n-2}	$= h$
A_{n-1}	$= \frac{1}{2}(x_n - x_{n-2})$	A_{n-1}	$= h$
A_n	$= \frac{1}{2}(x_n - x_{n-1})$	A_n	$= \frac{1}{2}h$

Figure 1.2: Coefficients for the Trapezoidal Rule

We can obtain a more accurate expression for the integral by treating pairs of consecutive intervals using a quadratic expression to represent the integrand over the complete two-interval area. The double sections can then be combined to obtain the integral over the full range.

Taking the three values of the abscissa to be (x_1, x_2, x_3) and the three values of the function $[f(x_1), f(x_2), f(x_3)]$ or (f_1, f_2, f_3), using Lagrange interpolation (Ref. I Sec. 25.2)

$$f(x) = \frac{(x_3-x_2)(x_2-x)(x_3-x)f_1+(x_3-x_1)(x_3-x)(x-x_1)f_2+(x_2-x_1)(x-x_2)(x-x_1)f_3}{(x_3-x_1)(x_2-x_1)(x_3-x_2)} \tag{1.5}$$

and integrating from x_1 to x_3 we find:

$$\int_{x_1}^{x_3} f(x)dx = \frac{(x_3-x_1)}{6}\left[\frac{(3x_2-2x_1-x_3)f_1}{x_2-x_1}+\frac{(x_3-x_1)^2 f_2}{(x_2-x_1)(x_3-x_2)}+\frac{(2x_3+x_1-3x_2)f_3}{x_3-x_2}\right]. \tag{1.6}$$

For the case of equal intervals the formula simplifies considerably:

$$\int_0^{2h} f(x)dx = \frac{h}{3}(f_1+4f_2+f_3). \tag{1.7}$$

We can now rearrange the series to obtain the coefficients of f_i by looking at the contributions to the coefficient of the function at each node. Note that for the points which fall on the boundary between two sections the function value contributes to the integral on each side and hence there are two contributions to the coefficient of that function value. Placing alternate contributions from the formula above and below the line of nodal points, we obtain the chart given in Figure 1.3.

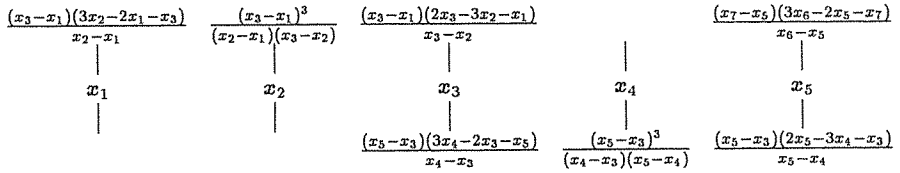

Figure 1.3: Contributions to the Nodal Points

Adding the contributions from above and below the line gives the coefficients shown in Table 1.1.

We have implicitly assumed that the range of the integral is finite, or can be treated as such. By this last statement it is meant that the integrand can be assumed to decrease rapidly enough that the approximation

$$\int_0^\infty f(x)dx \approx \int_0^R f(x)dx \tag{1.8}$$

can be made without significant loss of precision. Finding the appropriate value of R in a given case requires a certain amount of judgement (and testing) but once found, the integral to be evaluated by quadrature is of finite extent. However, if R has been taken larger than necessary (out of prudence perhaps) then a large number of evaluations may be indicated in a region where the integrand contributes very little. There are special techniques for treating integrals of infinite range which will be developed in section 1.4. For the remainder of this section, and for section 1.3, we shall assume that the range of integration is finite with $a \le x \le b$.

As we have seen, the strategy used for Simpson's rule is to join together pairs of intervals to cover the entire integration range, requiring that the number of intervals be even and the number of points odd. We might consider taking larger numbers of of intervals together but the algebra is beginning to get a little complicated for the case of unequal intervals. Let us consider an alternate approach to the problem of finding better integration schemes.

For the trapezoidal rule we arranged the coefficients in such a manner that a linear function would be integrated exactly since the dotted and solid curves in Figure 1.1 would coincide in this case. For the three point formula we arranged to integrate a quadratic polynomial exactly, which is equivalent to integrating a constant, the first power and the second power of the independent variable. To generalize this point of view we write

$$\int_a^b f(x)dx = \sum_{i=1}^{n} A_i f_i. \tag{1.9}$$

	Unequal Intervals ($\times\frac{1}{6}$)	Equal Intervals	
A_1	$\frac{(x_3-x_1)(3x_2-2x_1-x_3)}{x_2-x_1}$	$\frac{1}{3}h$	
A_2	$\frac{(x_3-x_1)^3}{(x_2-x_1)(x_3-x_2)}$	$\frac{4}{3}h$	
A_3	$\frac{(x_3-x_1)(2x_3-3x_2-x_1)}{x_3-x_2} - \frac{(x_5-x_3)(2x_3-3x_4+x_5)}{x_4-x_3}$	$\frac{2}{3}h$	
$\vdots$	$\vdots$	$\vdots$	
A_i	$\frac{(x_{i+1}-x_{i-1})^3}{(x_i-x_{i-1})(x_{i+1}-x_i)}$	$\frac{4}{3}h$	i even
A_i	$\frac{(x_i-x_{i-2})(2x_i-3x_{i-1}+x_{i-2})}{x_i-x_{i-1}} - \frac{(x_{i+2}-x_i)(2x_i-3x_{i+1}+x_{i+2})}{x_{i+1}-x_i}$	$\frac{2}{3}h$	i odd
$\vdots$	$\vdots$	$\vdots$	$\vdots$
A_n	$\frac{(x_n-x_{n-2})(2x_n-3x_{n-1}+x_{n-2})}{x_n-x_{n-1}}$	$\frac{1}{3}h$	n must be odd

Table 1.1: Coefficients for Simpson's Rule

This expression will be our basic starting point for deriving approximations for integrals. We will determine the values of the coefficients (and the points x_i) from conditions that this expression be exact for certain powers of x. If we wish to derive a formula to integrate the first $m+1$ powers of x exactly we have the following set of equations,

Power	Sum	Integral	Exact Result
0	$\sum_1^n A_i x_i^0$	$= \int_a^b x^0 dx$	$= b-a$
1	$\sum_1^n A_i x_i^1$	$= \int_a^b x^1 dx$	$= \frac{b^2-a^2}{2}$
2	$\sum_1^n A_i x_i^2$	$= \int_a^b x^2 dx$	$= \frac{b^3-a^3}{3}$
3	$\sum_1^n A_i x_i^3$	$= \int_a^b x^3 dx$	$= \frac{b^4-a^4}{4}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
m	$\sum_1^n A_i x_i^m$	$= \int_a^b x^m dx$	$= \frac{b^{m+1}-a^{m+1}}{m+1}$

(1.10)

where, of course, $m+1 \le n$.

For two points in a segment, with $a = -h/2$ and $b = h/2$, we have:

$$\begin{aligned} A_1 + A_2 &= h \\ -A_1\tfrac{h}{2} + A_2\tfrac{h}{2} &= 0 \quad \rightarrow \quad A_1 = A_2 \end{aligned}$$

thus $A_1 = \frac{h}{2} = A_2$ and the result is one segment of the trapezoidal rule.

For three points in a segment ($a = -h$, $b = h$; $x_1 = -h$, $x_2 = 0$ and $x_3 = h$) Eqs. 1.10 become:

$$\begin{aligned} A_1 + A_2 + A_3 &= 2h \\ -A_1 h + A_3 h &= 0 \quad \rightarrow \quad A_1 = A_3 \\ A_1 h^2 + A_3 h^2 &= \tfrac{2}{3}h^3 \end{aligned}$$

so that: $2A_1 = \frac{2}{3}h$ and

$$A_1 = \frac{1}{3}h, \qquad A_2 = \frac{4}{3}h, \qquad A_3 = \frac{1}{3}h \tag{1.11}$$

recovering the coefficients for Simpson's rule.

The set of coefficients $\{A_i\}$ are determined uniquely as the solution to a set of linear equations corresponding to a specified set of points $\{x_i\}$. Because of the form of the coefficients of the A_i in Eqs. 1.10 (powers of the x_i) the solution to the set of equations is guaranteed to exist if the x_i are unique.

Following is a program INTFOR which will be used to generate and study integration schemes. It provides the solution to this system of equations for a given set of points at which the function is to be evaluated. In the manner that it is presented here, the weighting schemes for any (modest) number of points with equal spacing is generated. However, the spacing of the nodes of the independent variable is arbitrary so that a set of weights for any collection of points could also be obtained. It is only necessary to change the loop defining the values of X(I) in order to generalize the program. Thus, if one were constrained to use data at fixed independent variable values, the points could be input to obtain the best weighting scheme to evaluate the integral.

The program calls the subroutine SGEFS which is a standard solver for linear systems. We will study the technique for such solutions in Chapter 5. If the routine is not available on your machine it will be necessary to replace it with another linear system solver.

```
C program to solve eqs. 1.10
C x contains the points of the independent variable
C v contains the matrix consisting of powers of x
C c contains the right hand side
c ca contains the capital a, i.e. the weights
```



```
      DIMENSION V(0:19,20),X(20),C(0:20),WORK(20),IWORK(20)
     1 ,Y(0:19,20),CA(0:19)
      B=1.              ! set up limits
      A=-1.
      N=2               ! number of equations
      H=(B-A)/FLOAT(N-1)    ! interval size h
      DO 1 I=1,N
      X(I)=A-H+I*H          ! equal spaced points
      V(0,I)=1.             ! first row of matrix
      Y(0,I)=1.             ! and save a copy
    1 CONTINUE
      DO 2 K=1,N-1
      DO 2 I=1,N
      V(K,I)=X(I)**K        ! make rest of matrix
      Y(K,I)=V(K,I)         ! and a copy
    2 CONTINUE
      DO 3 K=0,N-1
      C(K)=(B**(K+1)-A**(K+1))/FLOAT(K+1)  ! right hand side of eqs.
    3 CONTINUE
      DO 4 K=0,N-1    ! getting ready to call linear solver
    4 CA(K)=C(K)      ! answer will come out where rhs goes in
      CALL SGEFS(V,20,N,CA,0,WORK,IWORK)  ! solve N x N system
      DO 5 I=0,N-1
      PRINT 6,CA(I)/H,(Y(I,K),K=1,N),C(I),X(I+1)
    5 CONTINUE
    6 FORMAT(F8.4,12F6.1)
      DO 8 K=0,8     ! now integrate and check monomials up to 8
      SUM=0.
      DO 9 I=0,N-1
      IF (K.NE.0) TEM=X(I+1)**K
      IF (K.EQ.0) TEM=1.
    9 SUM=SUM+CA(I)*TEM
      PRINT 10,K,SUM,(B**(K+1)-A**(K+1))/FLOAT(K+1)
   10 FORMAT(I5,5F10.2)
    8 CONTINUE
      STOP
      END
```

Since we can transform from an arbitrary independent variable $a \leq t \leq b$ to the variable $-1 \leq x \leq 1$ by

$$x = \frac{2t - a - b}{b - a} \tag{1.12}$$

there is no loss of generality in taking $a = -1$ and $b = 1$. For this case Eqs. 1.10 become:

$$\sum_{i=1}^{n} A_i x_i^k = \begin{cases} 0 & \text{k odd} \\ \frac{2}{k+1} & \text{k even} \end{cases}$$

or

$$\begin{aligned} A_1 + A_2 + \ldots + A_n &= 2 \\ A_1 x_1 + A_2 x_2 + \ldots + A_n x_n &= 0 \\ A_1 x_1^2 + A_2 x_2^2 + \ldots + A_n x_n^2 &= \tfrac{2}{3} \\ A_1 x_1^3 + A_2 x_2^3 + \ldots + A_n x_n^3 &= 0 \\ \vdots \qquad\qquad\qquad & \quad \vdots \end{aligned}$$

Thus, given n distinct points, we can always satisfy the equations for n powers of x (x^0 through x^{n-1}) so that all monomials through order $n-1$ are integrated exactly. It is natural to ask if there exists an optimal choice of the $\{x_i\}$ to satisfy a maximum number of equations? The answer to this question is yes, and Section 1.3 develops the solution to this problem. Before attacking the general problem, however, we can examine some small systems to find the answer to this question for special cases in order to gat a feeling for how the technique works.

Consider the system of equations which arise for two points symmetrically positioned about the origin ($x_2 = -x_1$) but *not*, in general, at $(-1, +1)$ or $(-h, +h)$. In other words we consider a two-point scheme but with the two points *not* on the edge of the interval.

$$\begin{aligned} A_1 + A_2 &= 2 \\ A_1 x_1 + A_2 x_2 &= 0 \\ A_1 x_1^2 + A_2 x_2^2 &= \tfrac{2}{3} \\ A_1 x_1^3 + A_2 x_2^3 &= 0 \end{aligned}$$

All equations for odd powers of x are satisfied by $A_1 = A_2$. From the first equation we have $A_1 = A_2 = 1$ and from the third:

$$2A_1 x_1^2 = \frac{2}{3} \rightarrow x_1^2 = \frac{1}{3} \rightarrow x_1 = \pm\frac{1}{\sqrt{3}}$$

Thus a better scheme than the trapezoid rule would have equal weighting, h, with the nodes located at the points (assuming an integration range starting at zero):

$$(1 - \frac{1}{\sqrt{3}})h,\ (1 + \frac{1}{\sqrt{3}})h,\ (3 - \frac{1}{\sqrt{3}})h,\ (3 + \frac{1}{\sqrt{3}})h,\ \ldots$$

1.2 Orthogonal Polynomials

We will now develop some mathematical properties that will be needed in the next section.

1.2.1 Orthogonal Polynomials in the Interval $-1 \leq x \leq 1$

Let us suppose that we wish to construct a complete set of polynomials $P_n(x)$ which are orthogonal in the range $-1 \leq x \leq 1$, that is,

$$\int_{-1}^{1} P_n(x) P_{n'}(x) dx = 0 \text{ for } n \neq n'. \tag{1.13}$$

Each polynomial will be labeled by the subscript n denoting the highest power of x that it contains. While we can say immediately that $P_0(x)$ is a constant, we need another condition (beyond those already given) to determine its value. More generally each polynomial will have an additional condition (the normalization condition) which must be specified separately. We will take as this normalization condition* :

$$P_n(1) = 1 \tag{1.14}$$

so that $P_0(x) = 1$. Since $P_1(x)$ will consist of a constant and a linear term and

$$\int_{-1}^{1} x dx = 0,$$

the constant term must vanish to satisfy the orthogonality condition:

$$\int_{-1}^{1} P_0(x) P_1(x) dx = 0,$$

making P_1 proportional to x. The normalization condition requires that $P_1(x) = x$. To generalize, polynomials with even order will contain only even powers of x and those with odd order will contain only odd powers. The remainder of the polynomials can be calculated using Eqs. 1.13 and 1.14. Since the orthogonality condition holds (in particular) for $n' < n$, if we assume that all polynomials of order $n' < n$ are known, then Eq. 1.13 provides n conditions to determine the polynomial for n. There being $n + 1$ coefficients in the general expansion:

$$P_n(x) = \sum_{m=0}^{n} a_{n,m} x^m \tag{1.15}$$

*There have been a number of conditions used over the years but this one seems to be the most common at the present time.

the one additional normalization condition provides the needed information to determine each polynomial.

As an example of this procedure, let us calculate $P_2(x)$. We know that it must have the form

$$P_2(x) = a + bx + cx^2$$

where a, b and c are unspecified constants to be determined from the conditions 1.13 and 1.14. Since $P_2(x)$ is an even function (n is even) we also know that b=0[†]. Using the orthogonality condition with P_0:

$$\int_{-1}^{1} dx P_0(x)P_2(x) = 0 = \int_{-1}^{1} dx(a + cx^2) = 2a + \frac{2}{3}c$$

we find

$$c = -3a$$

and hence

$$P_2(x) = a(1 - 3x^2).$$

Since $P_2(1) = 1$, $a = -\frac{1}{2}$ and

$$P_2(x) = \frac{1}{2}(3x^2 - 1). \tag{1.16}$$

One can (in principle) continue in this manner to generate as many polynomials as desired.

These are the Legendre[‡] polynomials and are very important functions in the physical sciences.

Eq. 1.15 could, of course, be inverted to obtain the powers of x expanded in terms of the Legendre polynomials:

$$x^m = \sum_{n=0}^{m} b_{m,n} P_n(x). \tag{1.17}$$

We can see from this expression that a given Legendre polynomial, $P_n(x)$, is orthogonal to all powers of x with an exponent less than n.

$$\int_{-1}^{1} dx x^m P_n(x) = 0 \quad \text{for} \quad m = 0, 1, \ldots, n-1 \tag{1.18}$$

[†]This is only a short cut, the integral for the orthogonality with $P_1(x)$ would force it to be zero anyway.

[‡]These polynomials bear the name of the famous French mathematician Adrien Marie LeGendre (1752–1833). Note that he wrote his name with a capital "G" and since neither in English nor French has this spelling been retained, one risks some confusion with the butcher and leader of the French revolution born in the same year, Louis Legendre (1752–1797).

The $P_n(x)$ can be obtained efficiently by the recursion relation,

$$(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x) \tag{1.19}$$

and the derivative $[P_n'(x) \equiv \frac{dP_n(x)}{dx}]$ is given by:

$$(1 - x^2)P_n'(x) = -nxP_n(x) + nP_{n-1}(x). \tag{1.20}$$

The integral of the square of $P_n(x)$ is given by:

$$\int_{-1}^{1} dx P_n^2(x) = \frac{2}{2n+1}. \tag{1.21}$$

The $P_n(x)$ have n zeros, i.e. solutions for x to the equation

$$P_n(x) = 0. \tag{1.22}$$

These zeros are all real and all lie within the region $-1 \leq x_i \leq 1$.

Clearly a polynomial (or Taylor's series) approximation to any function can be rewritten as a series of Legendre polynomials. To obtain the coefficients, f_n, for the expansion of an arbitrary function in $P_n(x)$:

$$F(x) = \sum_{n=0}^{\infty} f_n P_n(x) \tag{1.23}$$

it is only necessary to multiply Eq. 1.23 by $P_m(x)$ and integrate from -1 to 1.

$$\int_{-1}^{1} dx F(x)P_m(x) = \sum_{n=0}^{\infty} f_n \int_{-1}^{1} P_n(x)P_m(x) = \frac{2}{2m+1} f_m,$$

leading to the general relation:

$$f_n = \frac{2n+1}{2} \int_{-1}^{1} dx F(x)P_n(x). \tag{1.24}$$

Of course the product of two Legendre polynomials (of the same argument) is itself expressible as a series of Legendre polynomials:

$$P_n(x)P_{n'}(x) = \sum_{m=0}^{n+n'} G_m^{n,n'} P_m(x). \tag{1.25}$$

The index, m, takes on even or odd values only, depending on whether $n + n'$ is even or odd. Here $G_m^{n,n'}$ (often known as Gaunt's integral) is given by:

$$G_m^{n,n'} = \frac{2m+1}{2} \int_{-1}^{1} P_m(x)P_n(x)P_{n'}(x)dx = \left[C_{n,n',m}^{0,0,0}\right]^2 \tag{1.26}$$

where the $C^{0,0,0}_{n,n',m}$ are the Clebsch-Gordan coefficients (Ref. I sec. 27.90). We will encounter these coefficients again in Chapter 10.

A physical quantity for which the expansion in Legendre polynomials is very natural is the scattering cross section. If no direction in space is defined, other than that of the incident and final particles, the cross section can be only a function of even powers of the scattering angle, θ, (due to azimuthal symmetry), and thus can be expressed as a function of $\cos\theta$ so that:

$$\sigma(\cos\theta) = \sum_{n=0}^{\infty} \sigma_n P_n(\cos\theta). \tag{1.27}$$

The integrated cross section

$$\sigma_I \equiv \int d\Omega \sigma(\cos\theta) \tag{1.28}$$

$$= \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta \sigma(\cos\theta) = 2\pi \int_{-1}^{1} dx \sigma(x), \tag{1.29}$$

is given by $4\pi\sigma_0$. Note the transformation $\sin\theta d\theta = -d\cos\theta = -dx$, for $x \equiv \cos\theta$.

1.2.2 General Orthogonal Polynomials

While the Legendre polynomials are very well adapted for representing functions in a finite interval, they are less suitable for ranges extending to infinity. It is possible to create a more efficient scheme for representing functions in those cases where there is a known dominant behavior for large values of the independent variable. These considerations suggest the generalization of the definition of an orthogonal polynomial used in the last section to:

$$\int_a^b w(x)\mathcal{P}_n(x)\mathcal{P}_{n'}(x)dx = 0 \quad \text{for} \quad n \neq n', \tag{1.30}$$

where $w(x)$ is a weighting function. For each form of $w(x)$ and range [a,b], a set of polynomials can be constructed as was done in the preceding section. Of course some weighting functions are more useful than others. A particularly valuable one is $w(x) = e^{-x}$ in the interval $[0, \infty]$. This choice leads to the Laguerre polynomials,

$$L_n(x) \equiv \sum_{m=0}^{n} \ell_{n,m} x^m. \tag{1.31}$$

For this case the normalization condition is given by fixing the coefficient of the highest power of x,

$$\ell_{n,n} = \frac{(-1)^n}{n!} \tag{1.32}$$

which also gives

$$\int_0^{\infty} w(x) L_n^2(x) = 1. \tag{1.33}$$

The recursion relation is:

$$(n+1)L_{n+1}(x) = (2n+1-x)L_n(x) - nL_{n-1}(x) \tag{1.34}$$

and the derivative is given by:

$$xL_n'(x) = nL_n(x) - nL_{n-1}(x). \tag{1.35}$$

There is a plethora of such orthogonal polynomials and the reader will find a summary of their properties in Ref. I, Sec. 22.

1.3 Gaussian Integration

The seeming digression of the previous section was made in order to prepare the way for the general solution to the problem (outlined at the end of section 1.1) of finding a maximally efficient integration scheme. We now rewrite equations 1.10 in the form:

$$\begin{array}{lll}
\sum_1^n A_i x_i^0 & -\int_a^b x^0 dx & = 0 \\
\sum_1^n A_i x_i^1 & -\int_a^b x^1 dx & = 0 \\
\sum_1^n A_i x_i^2 & -\int_a^b x^2 dx & = 0 \\
\vdots & \vdots & \vdots \\
\sum_1^n A_i x_i^{n-1} & -\int_a^b x^{n-1} dx & = 0 \\
\sum_1^n A_i x_i^n & -\int_a^b x^n dx & = Z_0(x_1, x_2, \ldots, x_n) \\
\sum_1^n A_i x_i^{n+1} & -\int_a^b x^{n+1} dx & = Z_1(x_1, x_2, \ldots, x_n) \\
\vdots & \vdots & \vdots \\
\sum_1^n A_i x_i^{n+k} & -\int_a^b x^{n+k} dx & = Z_k(x_1, x_2, \ldots, x_n) \\
\vdots & \vdots & \vdots
\end{array} \tag{1.36}$$

where we have assumed that the A_i have been chosen (for a fixed set x_i) so that the r.h.s. of the first n equations is zero, meaning that the first $n-1$ powers are integrated exactly. As we saw in Section 1.1 this is always possible for any set of independent

x_i. Starting with the n^{th} power, the right hand side of each equation will not, in general, be zero but instead some quantity which we will call Z_k, that depends on the selection of the points $\{x_i\}$. We will now attempt to choose the points $\{x_i\}$ such that $Z_0(x_1, x_2, \ldots, x_n) = 0$.

By multiplying each equation by the coefficient of the Legendre polynomial, $P_n(x)$, of Eq. 1.15, corresponding to its power (i.e. the equation for x^0 by $a_{n,0}$, the equation for x^1 by $a_{n,1}$, etc.) and summing the resulting $n+1$ equations (powers 0 through n) we arrive at an expression for the quantity $a_{n,n}Z_0(x_1, x_2, \ldots, x_n)$ in terms of the Legendre polynomials.

$$\sum_{i=1}^{n} A_i P_n(x_i) - \int_{-1}^{1} dx P_n(x) = a_{n,n} Z_0(x_1, x_2, \ldots, x_n) \tag{1.37}$$

The *integral* on the left hand side of eq 1.37 is automatically zero (for $n > 0$) so the problem of forcing $Z_0(x_1, x_2, \ldots, x_n)$ to zero is reduced to choosing the x_i so that the *sum* is zero. Since the polynomial $P_n(x)$ has exactly n zeros in the range $-1 \le x \le 1$, we can satisfy the condition by taking the x_i to be those zeros.

Once we have made this choice we can examine the effect on the next few equations as well. While Z_0 has been made zero, the r.h.s. of next equation (with value Z_1) corresponding to the power $n+1$, may not be. If we multiply the equation corresponding to the first power by $a_{n,0}$, that for the second power by $a_{n,1}$ etc., we arrive at:

$$\sum_{i=1}^{n} A_i x_i P_n(x_i) - \int_{-1}^{1} dx x P_n(x) = a_{n,n} Z_1(x_1, x_2, \ldots, x_n), \tag{1.38}$$

since there is exactly one more power of x in each equation than in the previous case. The sum in eq 1.38 is again zero and the integral will also be zero, if $n > 1$, so that Z_1 is also zero. We can continue in this manner starting the $a_{n,0}$ at successively higher and higher powers, k, to obtain a sequence of equations:

$$\sum_{i=1}^{n} A_i x_i^k P_n(x_i) - \int_{-1}^{1} dx x^k P_n(x) = a_{n,n} Z_k; \quad k = 0, 1, \ldots. \tag{1.39}$$

The sum on the l.h.s. will be zero for any value of k since the $P_n(x_i)$ are all zero by definition of the x_i. The integral (and hence Z_k) will be zero only for $k < n$. Thus we can satisfy n additional equations, $k = 0, 1, \ldots, n-1$ or a total of $2n$. This is the best we could hope to do since there are only $2n$ parameters at our disposal (n values of A_i and n values of x_i). It only makes sense to take n even since the odd equations are satisfied anyway[§].

[§]In fact it was a little bit of a cheat to talk about reducing the Z_k for odd k to zero, since they were always zero. But then, just taking n even was enough to assure that the sum was zero.

For the more general integral approximation

$$\int w(x) f(x) dx = \sum A_i f(x_i) \tag{1.40}$$

where we wish to consider $f(x)$ as represented by an expansion in powers of x, the argument follows in the same way for the general orthogonal polynomials. It is only necessary to include the weight function in Eqs. 1.36.

$$\begin{array}{lll}
\sum_1^n A_i x_i^0 & -\int_a^b w(x) x^0 dx & = 0 \\
\sum_1^n A_i x_i^1 & -\int_a^b w(x) x^1 dx & = 0 \\
\sum_1^n A_i x_i^2 & -\int_a^b w(x) x^2 dx & = 0 \\
\vdots & \vdots & \vdots \\
\sum_1^n A_i x_i^{n-1} & -\int_a^b w(x) x^{n-1} dx & = 0 \\
\sum_1^n A_i x_i^n & -\int_a^b w(x) x^n dx & = Z_0(x_1, x_2, \ldots, x_n) \\
\sum_1^n A_i x_i^{n+1} & -\int_a^b w(x) x^{n+1} dx & = Z_1(x_1, x_2, \ldots, x_n) \\
\vdots & \vdots & \vdots \\
\sum_1^n A_i x_i^{n+k} & -\int_a^b w(x) x^{n+k} dx & = Z_k(x_1, x_2, \ldots, x_n) \\
\vdots & \vdots & \vdots
\end{array} \tag{1.41}$$

Multiplying by the coefficients of the polynomial, $b_{n,m}$, and summing as before we obtain the result for the first additional power (k=0):

$$\sum_{i=1}^{n} A_i \mathcal{P}_n(x_i) - \int_a^b dx w(x) \mathcal{P}_n(x) = b_{n,n} Z_0(x_1, x_2, \ldots, x_3). \tag{1.42}$$

Once again, the integral is zero due to orthogonality and the sum can be made zero by choosing the x_i to be the zeros of $\mathcal{P}_n(x)$. The extension to $n-1$ more powers follows in the same manner as before.

These integration schemes are known by the name of Gauss followed by the name of the corresponding polynomial.

1.3.1 Gauss-Legendre Integration

In this case the integration is more-or-less evenly weighted over a finite region. The points are spaced so as to integrate any polynomial up to power $2(n-1)$ as derived

above. The technique is well suited for the integral over the "θ" variable in spherical coordinates, but can be applied to any finite integration with the transformation 1.12. Some examples of its use can be found in the problems

1.3.2 Gauss-Laguerre Integration

For this case (corresponding to an exponential weighting function) the points are distributed such that there are more near the origin where the function is large, with wider and wider spacing for larger values of the independent variable. Note that there is no need to truncate the integral at some large value, R, as was discussed before. The method itself chooses the largest value needed.

Of course it is rare that one has exactly the factor e^{-x} in the integrand. However it is often possible to transform the function into this form, or something closely resembling it. Suppose, for a simple example, that we have:

$$\int_0^\infty dy e^{-ay} f(y). \tag{1.43}$$

In this case we can write this integral (with the transformation $x = ay$) as

$$\frac{1}{a}\int_0^\infty dx e^{-x} f(\frac{x}{a}) \tag{1.44}$$

which *is* in the form required.

The Gauss-Laguerre scheme can be used to integrate *any* function since we can write:

$$\begin{aligned}\int_0^\infty dy f(y) &= \int_0^\infty dy e^{-ay} e^{ay} f(y)\\ &= \frac{1}{a}\int_0^\infty dx e^{-x}\ \ e^x f\left(\frac{x}{a}\right)\\ &\approx \frac{1}{a}\sum_{i=1}^n A_i e^{x_i} f\left(\frac{x_i}{a}\right) = \frac{1}{a}\sum_{i-1}^n A_i' f\left(\frac{x_i}{a}\right).\end{aligned}$$

The coefficients A_i' are often tabulated along with the A_i (see Ref. I, Table 25.9).

While this last transformation is completely general, the resulting approximation to the integral is accurate only if $e^x f(\frac{x}{a})$ is slowly varying. The value of "a" can be chosen to best achieve this goal.
Consider the example;

$$f(y) = \frac{e^{-2y}}{1+y^2}$$

so that

$$e^x f(\frac{x}{a}) = \frac{e^x e^{-\frac{2x}{a}}}{1+(\frac{x}{a})^2}.$$

If we take $a = 2$ then

$$e^x f(\frac{x}{a}) = \frac{4}{4+x^2},$$

which is relatively smooth.

Integrals of the Gauss-Laguerre type have a special role in treating "non-local" operators. These operators have this name because the most elementary formulation would make them simply multiplicative, or local. As an example of this form of an operator let us take:

$$\mathcal{V}(\mathbf{r})\psi(\mathbf{r}) = \int d\mathbf{r}' V(\mathbf{r},\mathbf{r}')\psi(\mathbf{r}'). \tag{1.45}$$

Then V is a non-local operator which has a a local limit:

$$V(\mathbf{r},\mathbf{r}') \overset{local}{\rightarrow} V(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}'). \tag{1.46}$$

It has been very common to use a local approximation as a convenience (and because the physics is reducible to more familiar terms) but with present computers the more accurate non-local problem can be solved as easily. However we are faced with the problem of wanting to solve the non-local case while maintaining the ability to reduce to the local limit. Gauss-Laguerre integration can be very useful in this regard. Consider a typical form for

$$V(\mathbf{r},\mathbf{r}') = V(\mathbf{r})\frac{\alpha^3}{8\pi}e^{-\alpha|\mathbf{r}-\mathbf{r}'|} \tag{1.47}$$

so that

$$\mathcal{V}(\mathbf{r})\psi(\mathbf{r}) = V(\mathbf{r})\frac{\alpha^3}{8\pi}\int d\mathbf{r}' e^{-\alpha|\mathbf{r}-\mathbf{r}'|}\psi(\mathbf{r}'). \tag{1.48}$$

The normalization has been chosen so that the limit as α tends to infinity yields a δ-function. To see this consider

$$\begin{aligned}\lim_{\alpha\to\infty}\frac{\alpha^3}{8\pi}\int d\mathbf{r}' e^{-\alpha|\mathbf{r}-\mathbf{r}'|}f(\mathbf{r}') &= f(\mathbf{r})\lim_{\alpha\to\infty}\frac{\alpha^3}{8\pi}\int d\mathbf{r}' e^{-\alpha|\mathbf{r}-\mathbf{r}'|} = f(\mathbf{r})\lim_{\alpha\to\infty}\frac{\alpha^3}{8\pi}\int ds e^{-\alpha s}\\ &= f(\mathbf{r})\lim_{\alpha\to\infty}\frac{\alpha^3}{2}\int_0^\infty s^2 dr e^{-\alpha s} = \frac{f(\mathbf{r})}{2}\lim_{\alpha\to\infty}\int_0^\infty y^2 e^{-y} = f(\mathbf{r}).\end{aligned} \tag{1.49}$$

With the transformation, $\mathbf{r}' - \mathbf{r} = \mathbf{t}$, we have in Eq. 1.48:

$$= V(\mathbf{r})\frac{\alpha^3}{8\pi}\int dt e^{-\alpha t}\psi(\mathbf{r}+\mathbf{t}) = V(\mathbf{r})\frac{\alpha^3}{2}\int_0^\infty t^2 e^{-\alpha t}\frac{1}{4\pi}\int d\Omega_t\psi(\mathbf{r}+\mathbf{t}) \tag{1.50}$$

Taking the limit as $\alpha \to \infty$ (the local limit) is difficult for equally spaced schemes since the integrand is becoming more and more singular. Making the transformation $y = \alpha t$ helps a great deal,

$$\mathcal{V}(\mathbf{r})\psi(\mathbf{r}) = V(\mathbf{r})\frac{1}{2}\int_0^\infty dy y^2 e^{-y}\frac{1}{4\pi}\int d\Omega\psi(\mathbf{r}+\frac{\mathbf{y}}{\alpha}) \tag{1.51}$$

but, even in the limit of $\alpha = \infty$ so that the second integral is just $\psi(\mathrm{r})$, one is still integrating the exponential. In this limit the remaining integral will be exact with a 3-point or more Gauss-Laguerre scheme.

1.4 Special Integration Schemes

It is possible to generate integration schemes including information about particular functions. Adapting the integration to do the first n powers of the variable may not be the best possible strategy. Suppose that it is known that the functions to be integrated may be approximately expressed as the sum of n functions $h_i, \quad i = 1, 2, \cdots n$.

For example, if we believe that the integrand can be represented as a sum of two functions $h_1(x)$ and $h_2(x)$, we can write the following two equations by taking all odd weights equal and all even weights equal. In this case we have:

$$A_o \sum_{i\ odd} h_1(x_i) + A_e \sum_{i\ even} h_1(x_i) = \bar{h}_1 \tag{1.52}$$

$$A_o \sum_{i\ odd} h_2(x_i) + A_e \sum_{i\ even} h_2(x_i) = \bar{h}_2 \tag{1.53}$$

where $\bar{h}_1$ and $\bar{h}_2$ are the (assumed known) integrals of the functions over the range. From these two equations the two weights can be found.

More generally if we can take a number of points, M, which is a multiple, m, of n, then we can chose the points as:

$$\begin{array}{llllll} 1, & n+1, & 2n+1, & \cdots, & n(m-1)+1 & \text{to have weight } A_1 \\ 2, & n+2, & 2n+2, & \cdots, & n(m-1)+2 & \text{to have weight } A_2 \\ 3, & n+3, & 2n+3, & \cdots, & n(m-1)+3 & \text{to have weight } A_3 \\ & & \vdots & & & \\ n, & 2n, & 3n, & \cdots, & nm & \text{to have weight } A_n \end{array}$$

Then we have the n equations:

$$\sum_{\ell=1}^{n} A_\ell \sum_{j=0}^{m-1} h_i(x_{\ell+jn}) = \int_a^b h_i(x)dx. \tag{1.54}$$

Defining

$$\bar{H}_i^\ell = \sum_{j=0}^{m-1} h_i(x_{\ell+jn}); \quad \bar{h}_i = \int_a^b h_i(x)dx$$

the solution of

$$\sum_{\ell=1}^{n} A_\ell \bar{H}_i^\ell = \bar{h}_i; \quad i = 1, 2, \cdots n \tag{1.55}$$

gives the weights.

1.5 Principal Value Integrals

In a number of physics problems, notably double or multiple scattering calculations, it becomes necessary to evaluate principal value integrals numerically. In particular the integral being considered is of the form:

$$\int_0^\infty \frac{f(x)dx}{x - x_0}. \tag{1.56}$$

A mneumonic often used for the expression of this integral is

$$\frac{1}{x - x_0} = i\pi\delta(x - x_0) + P \tag{1.57}$$

which is intended to indicate,

$$\int_0^\infty \frac{f(x)dx}{x - x_0} = i\pi f(x_0) + P\int_0^\infty \frac{f(x)dx}{x - x_0} \tag{1.58}$$

where the prefix, P, means the principal value is to be taken. Note that the resulting integral is complex even though the integrand is real. We will see why below.

The definition of the principal value integral is

$$P\int_0^\infty \frac{f(x)dx}{x - x_0} \equiv \lim_{\epsilon\to 0}\left[\int_0^{x_0-\epsilon} \frac{f(x)dx}{x - x_0} + \int_{x_0+\epsilon}^\infty \frac{f(x)dx}{x - x_0}\right]. \tag{1.59}$$

This integral can be computed directly from the definition by constructing the nodal mesh such that the points are located symmetrically with respect to x_0 with the point at x_0 not included. However, this is inconvenient in many cases. For example, the integral might be an interior integral with the value of x_0 depending on the external integration variables.

Often a better way to compute the integral is as follows. Since $f(x)$ must tend toward zero for large x, choose some R such that, for $x > R$, $f(x)$ is negligible allowing the approximation

$$\int_0^\infty \frac{f(x)dx}{x - x_0} \approx \int_0^R \frac{f(x)dx}{x - x_0}. \tag{1.60}$$

We can now rewrite

$$\int_0^R \frac{f(x)dx}{x - x_0} = \int_0^R \frac{[f(x) - f(x_0)]\,dx}{x - x_0} + f(x_0)\int_0^R \frac{dx}{x - x_0} \tag{1.61}$$

$$= \int_0^R \frac{[f(x) - f(x_0)]\,dx}{x - x_0} + f(x_0)\ln\frac{R - x_0}{-x_0} \tag{1.62}$$

Since

$$\ln\frac{R-x_0}{-x_0} = \ln(-1) + \ln\frac{R-x_0}{x_0} = i\pi + \ln\frac{R-x_0}{x_0},$$

$$\int_0^R \frac{f(x)dx}{x-x_0} = \int_0^R \frac{[f(x)-f(x_0)]\,dx}{x-x_0} + f(x_0)\ln\frac{R-x_0}{x_0} + i\pi f(x_0). \qquad (1.63)$$

We note that the imaginary part of Eq. 1.58 arrises from the fact that the logarithm of a negative number is imaginary.

Hence we have recovered the form above with the δ-function and an explicit expression for the principal value integral which can be evaluated by numerical means since the integrand

$$\frac{[f(x)-f(x_0)]}{x-x_0}$$

is smooth around x_0, provided one does not try to evaluate it at exactly that point. Note, however, that this integrand falls off very slowly for large x so that the integral must be accurately calculated out to R. The integral does *not* have to be carried out to large enough values of x to obtain an accurate value of the "$\frac{1}{x}$" part to infinity, however, since the logarithmic term represents that integral. The trapezoidal rule is often adequate.

Problems

Problems marked with * are meant to be solved without the aid of a computer.

1. * Combine the two-interval (3 point) Simpson's-rule expression with the one-interval (2 point) trapezoidal-rule expression to obtain a set of three-interval (4 point) integration weights.

2. * Derive an evenly spaced 3-point integration scheme to integrate exactly in the interval $-1 \le x \le 1$: i) a constant, ii) x (and hence all odd powers) and iii) x^4. It will not integrate x^2 exactly in general. Take $x_1 = -1$, $x_2 = 0$ and $x_3 = 1$.

3. Find the symmetric positions of the points in a 3 point integration rule [$x_1 = -x_3, x_2 = 0$] (i.e. find x_3)

   a) using INTFOR by defining $x(2) = 0.$, $x(3) = xx$, $x(1) = -x(3)$ and varying xx until the fourth-power equation is satisfied,

   and

   b) analytically using the same logic.

4. * Find the explicit representation of $P_3(x)$ using the expressions for the first three Legendre polynomials:

   $$P_0(x) = 1; \qquad P_1(x) = x; \qquad P_2(x) = \frac{1}{2}(3x^2-1)$$

   and a) the normalization condition [$P_n(1) = 1$] and the orthogonality relationship

   $$\int_{-1}^{1} dx P_n(x) P_3(x) = 0 \qquad \text{for n=0,1,2}$$

   b) the recursion formula

   $$(n+1)P_{n+1} = (2n+1)xP_n - nP_{n-1}.$$