Chapter 3 Numerical Integration

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- **Why numerical integration?**

It can be used to calculate *derivatives*!

Cauchy's theorem:

$$\frac{f^{(n)}(z^*)}{n!} = \frac{1}{2\pi i}\int_C \frac{f(z)}{(z-z^*)^{n+1}}dz \ , \qquad n = 1, 2, \cdots$$

Mechanics: Simple pendulum problem, $\cdots$.

Statistical Physics: Partition function, thermal averages, $\cdots$

$$Z = \sum_i e^{-\beta E_i} \ , \qquad < A > = \frac{1}{Z}\sum_i A_i e^{-\beta E_i} \ , \quad \beta = \frac{1}{k_B T} \ .$$

E&M: Electric field, $\cdots$.

$$\mathrm{E}(\mathbf{r}) = \int d^3\mathbf{r}' \rho(\mathbf{r}') \frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3} \ .$$

Solid State Physics: Overlap integral

$$\int dV \phi^*(\mathbf{r}) \chi(\mathbf{x}-\mathbf{r}) \ .$$

Molecular integrals

$$\int\int dV_1 dV_2 \Phi_a^*(\mathbf{r}_1)\Phi_a(\mathbf{r}_1) \ \frac{1}{r_{12}} \ \Phi_b^*(\mathbf{r}_2)\Phi_b(\mathbf{r}_2) \ ,$$

$$\int\int dV_1 dV_2 \Phi_a^*(\mathbf{r}_1)\Phi_b(\mathbf{r}_1) \ \frac{1}{r_{12}} \ \Phi_a^*(\mathbf{r}_2)\Phi_b(\mathbf{r}_2) \ .$$

- **Pendulum Problem**

The equation of motion is

$$ml\frac{d^2\theta}{dt^2} = -mg\sin\theta \ . \tag{1}$$

For small θ, solution is easy

$$\theta(t) = \theta_0\sqrt{\frac{g}{l}}t, \quad \theta(t=0) = \theta_0. \tag{2}$$

For real system, we solve Eq. (1) as follows

$$\frac{1}{2}\left(\frac{d\theta}{dt}\right)^2 = \frac{g}{l}(\cos\theta - \cos\theta_0),$$

$$dt = \sqrt{\frac{l}{2g}}\frac{d\theta}{\sqrt{\cos\theta - \cos\theta_0}} \ . \tag{3}$$

$$T = 4\sqrt{\frac{l}{2g}}\int_0^{\theta_0}\frac{d\theta}{\sqrt{\cos\theta - \cos\theta_0}} \ . \tag{4}$$

Do $\sin x = \sin(\theta/2)/\sin(\theta_0/2)$(*change variable*), $\Rightarrow$

$$T = 4\sqrt{\frac{l}{g}}K(\sin\frac{\theta_0}{2}) \quad (numerical) \ ,$$

the *complete elliptic integral of the first kind.*

$$K(k) = \int_0^{\pi/2}\frac{dx}{\sqrt{1-k^2\sin^2 x}} = F(k, \frac{\pi}{2}) \ . \tag{5}$$

This integral *diverges* at $k = 1$.

The elliptic integrals are commonly used in many physics problems and they are tabulated in many reference books.

The elliptic integral of the first kind (Lagendre):

$$
\begin{aligned}
F(k,\phi) &= \int_0^{\phi} \frac{dx}{\sqrt{1-k^2\sin^2 x}} \\
&= \int_0^{\sin\phi} \frac{dx}{\sqrt{(1-x^2)(1-k^2x^2)}} \ . \qquad (6)
\end{aligned}
$$

The elliptic integral of the second kind:

$$
\begin{aligned}
E(k,\phi) &= \int_0^{\phi} dx\sqrt{1-k^2\sin^2 x} \\
&= \int_0^{\sin\phi} dx\sqrt{\frac{1-k^2x^2}{1-x^2}} \ . \qquad (7)
\end{aligned}
$$

The elliptic integral of the third kind:

$$
\begin{aligned}
H(h,k,\phi) &= \int_0^{\phi} \frac{dx}{(1+h\sin^2 x)\sqrt{1-k^2\sin^2 x}} \\
&= \int_0^{\sin\phi} \frac{dx}{(1+hx^2)\sqrt{(1-x^2)(1-k^2x^2)}} \qquad (8)
\end{aligned}
$$

There are other kinds of elliptic integrals.

Many integrals can be transferred into elliptic integrals.

- **Review**

Basic rules:

1. $\int dx(Af(x) + Bg(x)) = A\int dx f(x) + B\int dx g(x)$
2. $\int d\phi(x) F'[\phi(x)] = F[\phi(x)] + C$
3. $\int U dV = UV - \int V dU$

Common integrals:

1. Rational functions: $P(x)/Q(x)$, both $P(x)\&Q(x)$ are polynomials. They are all integrable in principle, either directly or write it as a linear combination of the following functions:
$$\frac{A}{x-a}, \frac{A}{(x-a)^k}, \frac{Ax+B}{ax^2+bx+c}, \frac{Ax+B}{(ax^2+bx+c)^k}$$
2. Let $R(u(x), v(x))$ be a function obtainable by finite number of the four operations, $+, -, \times, /$ with $u(x), v(x)$ and constants.
   (a) $\int dx R(\sin x, \cos x)$: set $t = tan(x/2)$.
   (b) $\int dx R(x, (\frac{ax+b}{cx+d})^{1/n})$: set $t = (\frac{ax+b}{cx+d})^{1/n}$.
   (c) $\int dx R(x, \sqrt{ax^2+bx+c})$: set $u = x + b/2a$, then
$$\int du R(u, \sqrt{u^2+k^2}), \quad u = ktan(t) \ .$$

$$\int duR(u, \sqrt{u^2 - k^2}), \quad u = k/sin(t) \ .$$

$$\int duR(u, \sqrt{k^2 - u^2}), \quad u = ksin(t) \ .$$

3. Integration Table

- **Definition and Objective**

<u>Definition:</u> if there exists a function $F(x)$ whose derivative is $f(x) = dF(x)/dx$, then the definite integral

$$I(f) = \int_a^b dx f(x) = F(b) - F(a) \ . \tag{9}$$

Most integrals cannot be evaluated by Eq. (9).

Let's divide the interval $[a, b]$ by many sub-intervals

$$x_i = a + ih, x_0 = a, x_n = b; \qquad i = 1, 2, \cdots, n \ ,$$

then the simplest approximation for the integral is

$$I(f) \approx h \times \sum_i^n f(x_i) \ . \tag{10}$$

Formally, we write

$$I(f) = \sum_i^n W_i f_i + E_n, \quad f_i = f(x_i) \ , \tag{11}$$

and E_n is the error of the algorithm.

Objective: to find best x_i and W_i such that $\Sigma_i^n W_i f_i$ could approximate $I(f)$ *effectively*.

The naive formula corresponds to $W_i = h$.

- **Trapezoid Rule**

Try two points approximation, i.e.,

$$I(f) \approx T = W_0 f_0 + W_1 f_1 \ .$$

We want this to be useful for *all* integrals, and so we will require that it be *exact* for the simplest integrands, $f(x) = 1$ and $f(x) = x$.

$$\int_{x_0}^{x_1} dx 1 = x_1 - x_0 = W_0 + W_1 \ ,$$

and

$$\int_{x_0}^{x_1} dx x = \frac{x_1^2 - x_0^2}{2} = W_0 x_0 + W_1 x_1 \ .$$

Thus

$$W_0 = W_1 = \frac{x_1 - x_0}{2} = \frac{h}{2} \ .$$

<u>The trapezoid rule:</u>

$$\int_{x_0}^{x_1} dx f(x) = \frac{h}{2}(f_0 + f_1) - \frac{h^3}{12} f''(c), \ x_0 \leq c \leq x_1. \quad (12)$$

$$T_n(f) = h\left(\frac{f_0}{2} + f_1 + \cdots + f_{n-1} + \frac{f_n}{2}\right). \quad (13)$$

Equivalently, the trapezoid rule can be obtained by approximating integrand $f(x)$ by a linear polynomial

$$f(x) \approx P_1(x) = \frac{(b-x)f(a) + (x-a)f(b)}{b-a} \ .$$

Fig. 5.1

Fig. 5.2

- **Sequence of** h

  It is generally true that as h is decreased, numerical approximation to $I(f)$ becomes more accurate. Is it matter how do we decrease h?

  If n is doubled repeatedly, then the function values used in each $T_{2n}(f)$ will include all of the earlier function values used in the preceding $T_n(f)$.

Example 1 or Table 5.1

- **Simpson's Rule**

  Try three points approximation

Fig. 5.3

$$I(f) \approx S = W_0 f_0 + W_1 f_1 + W_2 f_2 \ .$$

$$\int_{x_0}^{x_2} dx 1 = x_2 - x_0 = W_0 + W_1 + W_2 \ ,$$

$$\int_{x_0}^{x_2} dx x = \frac{x_2^2 - x_0^2}{2} = W_0 x_0 + W_1 x_1 + W_2 x_2 \ ,$$

$$\int_{x_0}^{x_2} dx x^2 = W_0 x_0^2 + W_1 x_1^2 + W_2 x_2^2 \ .$$

<u>The Simpson's rule:</u>

$$\int_{x_0}^{x_2} dx f(x) = \frac{h}{3}(f_0 + 4f_1 + f_2) - \frac{h^5}{90} f^{(4)}(c) \ . \qquad (14)$$

$$\begin{aligned} S_n(f) &= \frac{h}{3}(f_0 + f_n) \qquad\qquad (n = 2k) \\ &+ \frac{4h}{3}(f_1 + f_3 + \cdots + f_{2k-1}) \\ &+ \frac{2h}{3}(f_2 + f_4 + \cdots + f_{2k-2}) \ . \end{aligned}$$

Equivalently,

$$
\begin{aligned}
f(x) \approx P_2(x) &= \frac{(x-b)(x-c)}{(a-b)(a-c)} f(a) \\
&+ \frac{(x-c)(x-a)}{(b-c)(b-a)} f(b) + \frac{(x-a)(x-b)}{(c-a)(c-b)} f(c) \, .
\end{aligned}
$$

Four points approximation $\Rightarrow$ <u>The Simpson's 3/8 rule:</u>

$$
\int_{x_0}^{x_3} dx \, f(x) = \frac{h}{3}(f_0+3f_1+3f_2+f_3) - \frac{3h^5}{80} f^{(4)}(c) \, . \tag{15}
$$

Five points approximation $\Rightarrow$ <u>The Boole's rule:</u>

$$
\begin{aligned}
\int_{x_0}^{x_4} dx \, f(x) &= \frac{2h}{45}(7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4) \\
&- \frac{8h^7}{945} f^{(6)}(c) \, .
\end{aligned} \tag{16}
$$

The process could be continued indefinitely.

$\vdots$

Example 1 (Sn) or
Table 5.2

- **Errors and Corrections**

  Do Taylor expansion for $f(x)$ about $x = a$ and $x = b$, and then perform integration:

$$\int_a^b dx f(x) = hf(a) + \frac{h^2}{2!}f^{'}(a) + \frac{h^3}{3!}f^{''}(a) + \frac{h^4}{4!}f^{'''}(a) + \frac{h^5}{5!}f^{(4)}(a)$$

$$\int_a^b dx f(x) = hf(b) - \frac{h^2}{2!}f^{'}(b) + \frac{h^3}{3!}f^{''}(b) - \frac{h^4}{4!}f^{'''}(b) + \frac{h^5}{5!}f^{(4)}(b)$$

  Do Taylor expansion for $f^{'}(x)$ about $x = a$ at $x = b$ and vice versa. Combine two to get

$$\begin{aligned} f^{''}(a) + f^{''}(b) &= \frac{2}{h}\left[f^{'}(b) - f^{'}(a)\right] - \frac{h}{2}\left[f^{'''}(b) - f^{'''}(a)\right] \\ &- \frac{h^2}{2}\left[f^{(4)}(b) + f^{(4)}(a)\right] + \cdots . \end{aligned}$$

  Do the same for $f^{'''}(x)$ to get

$$f^{(4)}(b) + f^{(4)}(a) = \frac{2}{h}\left[f^{'''}(b) - f^{'''}(a)\right] + \cdots .$$

$$\begin{aligned} \int_a^b dx f(x) &= \frac{h}{2}\left[f(b) + f(a)\right] - \frac{h^2}{12}\left[f^{'}(b) - f^{'}(a)\right] \\ &+ \frac{h^4}{720}\left[f^{'''}(b) - f^{'''}(a)\right] + \cdots . \end{aligned}$$

<u>*Euler-McClaurin* integration rule:</u>

$$\int_{x_0}^{x_n} dx f(x) = h\left(\frac{f_0}{2} + f_1 + f_2 + f_{n-1} + \frac{f_n}{2}\right) + E_n$$

$$E_n = \frac{h^2}{12}\left[f^{'}(x_0) - f^{'}(x_n)\right] - \frac{h^4}{720}\left[f^{'''}(x_0) - f^{'''}(x_n)\right] + \cdots .$$

<u>Corrected trapezoid rule:</u>

$$I(f) \approx T_n(f) - \frac{h^2}{12}\left[f^{'}(b) - f^{'}(a)\right] \; .$$

Such correction will not perform well if $f(x)$ is not two times continuously differentiable on $[a, b]$.

Similar analysis for the Simpson's rule leads to

$$E_n^S(f) = I(f) - S_n(f) = -\frac{h^4(b-a)}{180} f^{(4)}(c_n) \; .$$

and we have <u>corrected Simpson's rule:</u>

$$I(f) \approx S_n(f) - \frac{h^4}{180}\left[f^{'''}(b) - f^{'''}(a)\right] \; .$$

Simpson's rule will not perform well if $f(x)$ is not four times continuously differentiable on $[a, b]$.

Some other numerical algorithms must be used.

Example 2 or
Table 5.3

Table 5.4 shows
Simpson's rule not
perform well

Richardson Extrapolation

Error estimation: $I - I_n = \dfrac{c}{n^p}$, $\quad n = \dfrac{b-a}{h}$.

Trapezoid: $p = 2$; Simpson's: $p = 4$. (*not always!*)

$$I - I_{2n} = \frac{c}{2^p n^p} \,, \quad 2^p[I - I_{2n}] = I - I_n \;.$$

$$I = \frac{2^p I_{2n} - I_n}{2^p - 1} \equiv R_{2n} \text{ , the improved estimate of } I$$

Richardson's error estimate

$$I - I_{2n} = R_{2n} - I_{2n} = \frac{I_{2n} - I_n}{2^p - 1} \;.$$

Extrapolation (Romberg Integration Scheme)

$$T_{m,k} = \frac{4^k T_{m,k-1} - T_{m-1,k-1}}{4^k - 1} \;.$$

$m(n = 2^m)$	$T_{m,0}$	$T_{m,1}$	$T_{m,2}$	$T_{m,3}$
0	$T_{0,0}$			
1	$T_{1,0}$	$T_{1,1}$		
2	$T_{2,0}$	$T_{2,1}$	$T_{2,2}$	
3	$T_{3,0}$	$T_{3,1}$	$T_{3,2}$	$T_{3,3}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

Example on page 157-158: (i) calculate ratio R_m,

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$$R_m = \frac{T_{m-1,0} - T_{m,0}}{T_{m,0} - T_{m+1,0}} = 4?$$

(ii) points where $f^{(k)}(x)$ is not analytical.

Periodic Integrands

$$f(x+\tau) = f(x), \quad -\infty < x < \infty \ .$$

Let $b - a = n\tau$, then $f^{(k)}(a) = f^{(k)}(b) \Rightarrow$ *the asymptotic error is zero.* (previous example)

The trapezoid rule is the preferred integration algorithm when we are dealing with smooth periodic integrands.

- **Change of Variables/Improper Integrals**

This is a common trick used in all kinds of problems.

$$\int_0^\infty dx\, f(x) = \lim_{A\to\infty} \int_0^A dx\, f(x) \ .$$

$$\int_0^\infty = \int_0^a + \int_a^\infty = I_1 + I_2 \ .$$

Make variable change $x \to 1/y$ ($x \to (1+y)/(1-y)$),

$$I_2 = \int_0^{1/a} dy \frac{f(y^{-1})}{y^2} \ .$$

Other choices:

$$x \to \frac{1+y}{1-y}, \quad x \to \frac{y}{y-1}, \quad x \to e^{-y}, \quad etc.$$

Series expansion, subtract the singularity away,

integration by parts, etc.:

$$I = \int_0^\infty \frac{dx}{(1+x)\sqrt{x}} \cdots \ .$$

(example on page 166-168)

Print out book "A First Course in Computational Physics" pages 164-168.
Use the examples.

• Gaussian Integration

Minimax approximation of order n

$$max_{a \le x \le b} |f(x) - p_n(x)| = \rho_n(f) \ ,$$

where $p_n(x)$ is a polynomial of degree $\le n$.

n	$\rho_n(f)$	n	$\rho_n(f)$	n	$\rho_n(f)$
1	5.30E-2	4	4.63E-4	7	4.62E-7
2	1.79E-2	5	1.62E-5	8	9.64E-8
3	6.63E-4	6	7.82E-6	9	8.05E-9

$f(x) = e^{-x^2}$
$0 \le x \le 1$

A standard map:

$[a, b] \Rightarrow [-1, 1]$ by

$$\tilde{x} = -1 + 2\frac{x - a}{b - a} \ .$$

We want

$$I(f) = \int_{-1}^{1} dx f(x) \doteq I_n(f) = \sum_{i=1}^{n} w_i f(x_i)$$

and require that the nodes $\{x_1, \cdots, x_n\}$ *and weights* $\{w_1, \cdots, w_n\}$ *be chosen so that* $I_n(f) = I(f)$ *for all polynomials* $f(x)$ *of as large a degree as possible.*

1. $n = 1$, $\int_{-1}^{1} dx f(x) \doteq w_1 f(x_1)$

$$f(x) = 1 \Rightarrow 2 = w_1$$

$$f(x) = x \Rightarrow 0 = x_1$$

$$\int_{-1}^{1} dx f(x) \doteq 2f(0) \equiv I_1(f) \ .$$

2. $n = 2$, $\int_{-1}^{1} dx f(x) \doteq w_1 f(x_1) + w_2 f(x_2)$

$$f(x) = 1 \Rightarrow 2 = w_1 + w_2$$

$$f(x) = x \Rightarrow 0 = w_1 x_1 + w_2 x_2$$

$$f(x) = x^2 \Rightarrow \frac{2}{3} = w_1 x_1^2 + w_2 x_2^2$$

$$f(x) = x^3 \Rightarrow 0 = w_1 x_1^3 + w_2 x_2^3$$

$$w_1 = w_2 = 1, x_2 = -x_1 = \frac{1}{\sqrt{3}}$$

$$\int_{-1}^{1} dx f(x) \doteq f(-\frac{1}{\sqrt{3}}) + f(\frac{1}{\sqrt{3}}) \equiv I_2(f) \ .$$

3. $n > 2$ There are $2n$ unspecified coefficients so we force the integration formula to be exact for the $2n$ monomilas

$$f(x) = 1, x, x^2, \cdots, x^{2n-1} \ .$$

This leads to a set of $2n$ *nonlinear* equations, a formidable task!

$\boxed{\text{Table 5.9 for periodic function. Not as good for Trapezoidal}}$

$\boxed{\text{Table 5.7}}$ $\boxed{\text{Table 5.8}}$

Gauss-Legendre Integration

With the use of the *theory of orthogonal polynomials*, one can determine those nodes and weights.

The nodes $\{x_1, \cdots, x_n\}$ are the *zeros* of the *Legendre polynomial* of degree n on the interval $[-1, 1]$.

The weights $\{w_1, \cdots, w_n\}$ can be obtained from the following *linear equations*:

$$\sum_{i=1}^{n} w_i x_i^k = \begin{cases} \frac{2}{k+1} & k \ even \\ 0 & k \ odd \end{cases} \qquad k = 0, 1, \cdots, 2n-1.$$

Gauss-Laguerre Integration

$$I = \int_0^\infty dx e^{-x} f(x) = \sum_{i=1}^{n} w_i f(x_i) \ .$$

These nodes and weights are tabulated, e.g., Tables 4.1 and 4.2.

A First ... Computational Physics Table 4.1 (page 177) Table 7.2 (p 181)

- **Multidimensional Integration**

$$I = \int_a^b dx \int_c^d dy f(x, y).$$

1. For rectangular region, it is easy:

$$I = \int_c^d dy F(y), \qquad F(y) = \int_a^b dx f(x, y).$$

or

$$I = \int_a^b dx G(x), \qquad G(x) = \int_c^d dy f(x, y).$$

2. For curved region, say $b : x = g(y)$,

$$I = \int_c^d dy F(y), \qquad F(y) = \int_a^{g(y)} dx f(x, y).$$

3. Try change of variables.

The integration is much harder and time consuming.

Tabulated formulae (math handbooks)

$$I = \int dx dy f(x, y) = \sum_{i=1}^{n} w_i f(x_i, y_i) + R$$

$$I = \int dx dy dz f(x, y, z) = \sum_{i=1}^{n} w_i f(x_i, y_i, z_i) + R$$

- **Monte Carlo Integration**

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Sample Mean algorithm:

$$I_n = (b-a) < f >= (b-a)\frac{1}{n}\sum_{i=1}^{n} f(x_i)$$

You can think of $w_i = (b-a)/n$.

Hit or Miss algorithm:

$$I_n = A\frac{n_s}{n}$$

Error Estimation:

$$\sigma_n = \sqrt{\frac{1}{n}\sum f^2(x_i) - \left(\frac{1}{n}\sum f(x_i)\right)^2} / \sqrt{n-1}\ .$$

If the numerical goes as order n^{-k} in one dimension integration, then the error in d dimensions goes as $n^{-k/d}$. In contrast, Monte Carlo errors vary as order $n^{-1/2}$ independent of d.

Importance Sampling:

$$\int_a^b dx\, f(x) = \int_a^b dx p(x)\frac{f(x)}{p(x)}\ .$$

Chapter 3 Review

Numerical Integration is Very Important!

– The trapezoid rule: $(h = (b-a)/n)$

$$\begin{aligned} T_n(f) &= h\left(\frac{f_0}{2} + f_1 + \cdots + f_{n-1} + \frac{f_n}{2}\right), \\ I(f) &\approx T_n(f) - \frac{h^2}{12}\left[f^{'}(b) - f^{'}(a)\right] (asymptotic) \ . \end{aligned}$$

– The Simpson's rule: $(h = (b-a)/n, n = 2k)$

$$\begin{aligned} S_n(f) &= \frac{h}{3}(f_0 + f_n) + \frac{4h}{3}(f_1 + f_3 + \cdots + f_{2k-1}) \\ &+ \frac{2h}{3}(f_2 + f_4 + \cdots + f_{2k-2}), \\ I(f) &\approx S_n(f) - \frac{h^4}{180}\left[f^{'''}(b) - f^{'''}(a)\right] \ . \end{aligned}$$

– Romberg Integration Scheme (Extrapolation)

$$T_{m,k} = \frac{4^k T_{m,k-1} - T_{m-1,k-1}}{4^k - 1} \ .$$

– Change of Variables.

– Gaussian Integration.

– Monte Carlo Integration.

Example 1. Three integrations:

$$
\begin{aligned}
I_1 &= \int_0^1 dx e^{-x^2} = 0.74682413281234 \\
I_2 &= \int_0^4 \frac{dx}{1+x^2} = arctan(4) = 1.3258176636680 \\
I_3 &= \int_0^{2\pi} \frac{dx}{2+\cos(x)} = \frac{2\pi}{\sqrt{3}} = 3.6275987284684
\end{aligned}
$$

	$T_n - I_1$		$T_n - I_2$		$T_n - I_3$	
n	Error	Ratio	Error	Ratio	Error	Ratio
2	1.55E-2		-1.33E-1		-5.61E-1	
4	3.84E-3	4.02	-3.59E-3	37.00	-3.76E-2	14.9
8	9.59E-4	4.01	5.64E-4	-6.37	-1.93E-4	195.0
16	2.40E-4	4.00	1.44E-4	3.92	-5.19E-9	37600.0
32	5.99E-5	4.00	3.60E-5	4.00		
64	1.50E-5	4.00	9.01E-6	4.00		
128	3.74E-6	4.00	2.25E-6	4.00		

	$S_n - I_1$		$S_n - I_2$		$S_n - I_3$	
n	Error	Ratio	Error	Ratio	Error	Ratio
2	-3.56E-4		8.66E-2		-1.26	
4	-3.12E-5	11.4	3.95E-2	2.20	1.37E-1	-9.2
8	-1.99E-6	15.7	1.95E-3	20.3	1.23E-2	11.20
16	-1.25E-7	15.9	4.02E-6	485.	6.43E-5	191.0
32	-7.79E-9	16.0	2.33E-8	172.	1.71E-9	37600
64	-4.87E-10	16.0	1.46E-9	16.0		
128	-3.04E-11	16.0	9.15E-11	16.0		

Example 2. Integral I_1. (Correction)

n	$I_1 - T_n$	E_n^T	CT_n	$I_1 - CT_n$	Ratio
2	1.545E-2	1.533E-2	0.746698561877	1.26E-4	
4	3.840E-3	3.823E-2	0.746816175313	7.96E-6	15.8
8	9.585E-4	9.580E-4	0.746823634224	4.99E-7	16.0
16	2.395E-4	2.395E-4	0.746824101633	3.12E-8	16.0
32	5.988E-5	5.988E-5	0.746824130863	1.95E-9	16.0
64	1.497E-5	1.497E-5	0.746824132690	2.22E-10	16.0
∞			0.746824132812		

Example 3. Integral:

$$I = \int_0^1 dx \sqrt{x} = \frac{2}{3} \ .$$

n	$I - S_n$	Ratio	$I - T_n$	$I - G_n$
2	2.860E-2		6.31E-2	-7.22E-3
4	1.012E-2	2.82	2.34E-2	-1.16E-3
8	3.587E-3	2.83	8.54E-3	-1.69E-4
16	1.268E-3	2.83	3.09E-3	-2.30E-5
32	4.485E-4	2.83	1.11E-3	-3.00E-6

f', f'', f''' does not exist at $x = 0$.

Integral I_1 by Gaussian Integration:

n	$I_1 - G_n$	$I_2 - G_n$	$I_3 - G_n$
2	2.29E-4	-2.33E-2	8.23E-1
3	9.55E-6	-3.49E-2	-4.30E-1
4	-3.35E-7	-1.90E-3	1.77E-1
5	6.05E-9	1.70E-3	-8.12E-2
6	-7.77E-11	2.74E-4	3.55E-2
7	8.60E-13	-6.45E-5	-1.58E-2
10		1.27E-6	1.37E-3
15		7.40E-10	-2.33E-5
20			3.96E-7

Error Function

Error function:

$$erf(x) = \frac{2}{\sqrt{\pi}} \int_0^x dt e^{-t^2}$$

Complementary error function:

$$erfc(x) \equiv 1 - erf(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty dt e^{-t^2}$$

The functions have the following

limiting values and symmetries:

$$erf(0) = 0 \quad erf(\infty) = 1 \quad erf(-x) = erf(x)$$

$$erfc(0) = 1 \quad erfc(\infty) = 0 \quad erfc(-x) = 2 - erfc(x)$$