Chapter 5

Numerical Integration

(數值積分法)

5.1 Definite Integral

Many techniques are described in calculus courses for the exact evaluation of integrals, but these techniques can seldom be used to evaluate the integrals that occur in real-life problems. Therefore, we need approximation methods for those physical-world problems.

回顧微積分中, 一函數 f 之不定積分(indefinite integral) 是求 f 的反導數:

$$\int f(x)\,dx = F(x) + C$$

其結果爲一函數集 (a family of functions). 其中函數 F 是 f 的反導數 (anti-derivative), 即 $F'(x) = f(x)$. C 是積分常數. 而函數 f 之定積分(definite integral) 是 f 在一固定區間 $[a, b]$ 之積分:

$$\int_a^b f(x)\,dx = [F(x)]_a^b = F(b) - F(a)$$

其結果爲一實數值. 依據微積分基本定理, 我們必須先求得其反導數 F 再代入其上限與下限. 然而某些積分很難求得一明顯的反導數. 例如: 欲求

$$\int_0^1 e^{x^2}\,dx$$

之值, 我們很難找到 e^{x^2} 之反導數. 因此我們只能尋求數值積分法(numerical integration) 以求其數值解.

★ 求定積分之近似值的公式通常稱爲 Rules(法則), 因此求定積分之數值方法又叫做 quadrature rules. (註: quadrature 之意思很多, 在數學上主要之意思爲 "用數值方法求曲線下之面積的進似值".)

常見的數值積分法有

- Basic quadrature rules
- Gaussian quadrature rule
- Romberg algorithm
- Adaptive algorithms

5.2 Basic Quadrature Rules

In this section, we shall introduce the basic quadrature rules:

- Midpoint rule
- Trapezoidal rule
- Simpson's rule

Midpoint Rule

Definition of 黎曼積分(Riemann Integral):

設一非負函數 f 在閉區間 $[a,\, b]$ 連續且 P 爲 $[a,\, b]$ 上之任一分割 (partition) 表成:

$$P = \{a = x_0 < x_1 < ... < x_n = b\}.$$

點 $x_0, x_1, ..., x_n$ 將區間 $[a,\, b]$ 分爲 n 個子區間 $[x_{i-1},\, x_i]$, 其長度爲 $\Delta x_i = x_i - x_{i-1}$. 取 x_i^* 爲子區間 $[x_{i-1},\, x_i]$ 上任一點, 則 f 在 $[a,\, b]$ 上之黎曼和 (Riemann Sum) 定義爲

$$R(f;\, P) = \sum_{i=1}^{n} f(x_i^*)\Delta x_i \approx \int_a^b f(x)\, dx.$$

若定義 $||P|| = \max\{\Delta x_i | 0 \le i \le n-1\}$, 稱爲 P 的模 (norm). 則 f 在區間 $[a,\, b]$ 之定積分定義爲

$$\int_a^b f(x)\,dx = \lim_{||P|| \longrightarrow 0} \sum_{i=1}^{n} f(x_i^*)\Delta x_i.$$

★ 應用黎曼和來求定積分之近似値的方法稱爲矩形法(Rectangular Rule). 依 x_i^* 之取法, 矩形法又可分爲:

- 右點法則(RRR–right-rectangle rule): 取 x_i^* 爲 $[x_{i-1},\, x_i]$ 之右端點, 即 $x_i^* = x_i$.
- 左點法則(LRR–left-rectangle rule): 取 x_i^* 爲 $[x_{i-1},\, x_i]$ 之左端點, 即 $x_i^* = x_{i-1}$.
- 中點法則(MPR–midpoint rule): 取 x_i^* 爲 $[x_{i-1},\, x_i]$ 之中點, 即 $x_i^* = (x_{i-1} + x_i)/2$.

矩形法中最常用的爲中點法, 其基本公式爲:

$$\int_{x_{i-1}}^{x_i} f(x)\,dx \approx f\left(\frac{x_{i-1}+x_i}{2}\right)\Delta x_i, \quad \Delta x_i = x_i - x_{i-1}.$$

定理 **1. Midpoint Rule**

If $f \in C^2[a,b]$, then a number ξ in (a,b) exists with

$$\int_a^b f(x)\,dx = (b-a)f\left(\frac{a+b}{2}\right) + \frac{f''(\xi)}{24}(b-a)^3. \qquad (5.1)$$

The error term $E = \frac{h^3}{24} f''(\xi)$ with $h = b - a$.

在實際應用上, 我們通常取 P 爲等分割 (uniform partition), 即 $\Delta x_i = h = (b-a)/n$, $x_i = a + ih$, $0 \le i \le n$. 因此合成中點法 (the composite midpoint rule), denoted as $M(f;\, P)$, 可表爲

$$\int_a^b f(x)\,dx \approx M(f;\, P) = h\sum_{i=1}^{n} f\left(\frac{x_{i-1}+x_i}{2}\right). \qquad (5.2)$$

Trapezoidal Rule

若欲 estimate $\int_a^b f(x)dx$ 之值. 同樣地, 將 $[a,\, b]$ 分割成 n 個子區間. 設 P 是 $[a,\, b]$ 之一分割:

$$P = \{a = x_0 < x_1 < \ldots < x_n = b\}$$

對每一子區間 $[x_{i-1},\, x_i]$ 取梯形面積來近似曲線下之面積:

$$\text{梯形面積} = \text{底邊長} \times \text{平均高 (左右兩端點之函數的平均值)}$$

$$\begin{aligned}\int_{x_{i-1}}^{x_i} f(x)\,dx \approx A_i &= (x_i - x_{i-1})\left[\frac{f(x_{i-1}) + f(x_i)}{2}\right]\\ &= \frac{1}{2}(x_i - x_{i-1})\left[f(x_{i-1}) + f(x_i)\right],\end{aligned}$$

which is the **basic trapezoid rule**. 即 $n = 1$ 時, 寫成如下定理:

定理 2. Trapezoidal Rule

If $f \in C^2[a,b]$, then a number ξ in (a,b) exists with

$$\int_a^b f(x)\,dx = (b-a)\left[\frac{f(a)+f(b)}{2}\right] - \frac{f''(\xi)}{12}(b-a)^3. \tag{5.3}$$

若分成 n 個子區間, 則所有梯形面積之總和為

$$\int_a^b f(x)\,dx \approx T(f;\, P) = \frac{1}{2}\sum_{i=1}^{n}(x_i - x_{i-1})[f(x_{i-1}) + f(x_i)] \tag{5.4}$$

which is called the **composite trapezoid rule**, denoted as $T(f;\, P)$.

Error of The Trapezoidal Rule

定理 3. *若 f'' exists 且連續在 $[a,\, b]$ 且 the composite trapezidal rule T 以 uniform spacing h to estimate the integral $I = \int_a^b f(x)\,dx$ 則存在某數 $\xi \in (a,b)$ 使得*

$$I - T = -\frac{1}{12}(b-a)h^2 f''(\xi) = O(h^2)$$

PROOF: (i) 首先證明當 $a = 0$, $b = 1$, $h = 1$ 時

$$\int_0^1 f(x)dx = \frac{1}{2}[f(0) + f(1)] - \frac{1}{12}f''(\zeta) \tag{5.5}$$

應用 Polynomial interpolation, let $p(x)$ be the polynomial of degree 1 that interpolates f at 0 and 1, 則

$$p(x) = f(0) + [f(1) - f(0)]x$$

and therefore

$$\int_0^1 p(x)dx = f(0) + \frac{1}{2}[f(1) - f(0)] = \frac{1}{2}[f(0) + f(1)] \tag{5.6}$$

By the error formula of the interpolating polynomial (Theorem 6 in Chapter 4), we have

$$f(x) - p(x) = \frac{1}{2}f''(\xi_x)x(x-1), \tag{5.7}$$

where ξ_x depends on x in $(0, 1)$. It follows that

$$\int_0^1 f(x)dx - \int_0^1 p(x)dx = \frac{1}{2}\int_0^1 f''(\xi_x)x(x-1)dx \tag{5.8}$$

That $f''(\xi_x)$ is continuous can be proved by solving Eq.(5.7). Notice that $x(x-1)$ 在 $[0, 1]$ 符號不變. 故 by Mean Value Theorem for Integerals, 存在一點 $x = s$

$$\begin{aligned}
\int_0^1 f''(\xi_x)x(x-1)dx &= f''(\xi_s)\int_0^1 x(x-1)dx \\
&= -\frac{1}{6}f''(\zeta)
\end{aligned}$$

其中 $\zeta = \xi_s$. By putting the above result and Eq.(5.8) back to Eq.(5.7), we have proved the Eq.(5.5).

Next, From Eq.(5.5), 應用變數變換將在 $[0, 1]$ 之積分轉換成 $[a, b]$ 之積分, 即可得 the basic trapezoidal rule

$$\int_a^b f(x)\,dx = \frac{b-a}{2}[f(a) + f(b)] - \frac{f''(\xi)}{12}(b-a)^3$$

令

$$\begin{aligned} x &= a+(b-a)t, \quad 0 \le t \le 1, \quad \text{則 } x \text{ 從 } a \text{ 到 } b \\ g(t) &= f(a+t(b-a)), \quad d(x) = (b-a)dt \\ \therefore g'(t) &= f'[a+t(b-a)](b-a) \\ \text{and } g''(t) &= f''[a+t(b-a)](b-a)^2. \end{aligned}$$

By Eq.(5.5),

$$\begin{aligned} \int_a^b f(x)dx &= (b-a)\int_0^1 f[a+t(b-a)]dt \\ &= (b-a)\int_0^1 g(t)dt \\ &= (b-a)\left\{\frac{g(0)+g(1)}{2} - \frac{1}{12}g''(\zeta)\right\} \\ &= \frac{b-a}{2}[f(a)+f(b)] - \frac{(b-a)^3}{12}f''(\xi). \end{aligned}$$

Here $\xi = a+\zeta(b-a)$ is in (a, b) and hence the error term $E = \frac{h^3}{12}f''(\xi)$ with $h = b-a$. ■

若將 $[a, b]$ 分割成 n 個等子區間, 即 $\Delta x_i = h = (b-a)/n, \forall i$. 應用公式 (4) 到 $[x_{i-1}, x_i]$ 得

$$\int_{x_{i-1}}^{x_i} f(x)dx = \frac{h}{2}[f(x_{i-1}) + f(x_i)] - \frac{1}{12}h^3 f''(\xi)$$

其中 $x_{i-1} < \xi_i < x_i$. 使用此結果於每一個子區間

$$\begin{aligned} \int_a^b f(x)\,dx &= \sum_{i=1}^n \int_{x_{i-1}}^{x_i} f(x)dx \\ &= \frac{h}{2}\sum_{i=1}^n [f(x_{i-1})+f(x_i)] - \frac{h^3}{12}\sum_{i=1}^n f''(\xi_i). \end{aligned}$$

The error term, 因 $h = (b-a)/n$, 可化簡爲

$$\begin{aligned} E = -\frac{h^3}{12}\sum_{i=1}^n f''(\xi_i) &= -\frac{b-a}{12}h^2\left[\frac{1}{n}\sum_{i=1}^n f''(\xi_i)\right], \\ &= -\frac{b-a}{12}h^2 f''(\zeta), \quad \text{for some } \zeta \in (a,b). \end{aligned}$$

Here we have used **the Intermidiate-Value Theorem of Continuous Functions** for the average $[1/n]\sum_{i=1}^{n} f''(\xi_i) = f''(\zeta)$ for some ζ in (a, b).

例題 **1.** 應用 *Taylor Series to represent the error in the basic trapezoidal rule by infinite series.*
解答：
The formula (5.3) is equivalent to

$$\int_a^{a+h} f(x)dx = \frac{h}{2}[f(a) + f(a+h)] - \frac{1}{12}h^3 f''(\xi)$$

令 $F(t) = \int_a^t f(x)dx$ 則 *Taylor series for* F *is*

$$F(a+h) = F(a) + hF'(a) + \frac{h^2}{2}F''(a) + \frac{h^3}{3!}F'''(a) + \cdots$$

由 *Fundamental Theorem of Calculus*, $F' = f$ *and* $F(a) = 0, F'' = f', F''' = f'', \cdots,$ 等等. 故

$$\int_a^{a+h} f(x)dx = hf(a) + \frac{h^2}{2}f'(a) + \frac{h^2}{3!}f''(a) + \cdots \tag{5.9}$$

$$f(a+h) = f(a) + hf'(a) + \frac{h^2}{2}f''(a) + \frac{h^3}{3!}f'''(a) + \cdots$$

加 $f(a)$ 於兩邊且乘以 $\frac{h}{2}$，得

$$\frac{h}{2}[f(a) + f(a+h)] = hf(a) + \frac{h^2}{2}f'(a) + \frac{h^3}{4}f''(a) + \cdots \tag{5.10}$$

由 *Eq.(5.9) and (5.10),* 得

$$\int_a^b f(x)dx - \frac{h}{2}[f(a) + f(a+h)] \;=\; -\frac{1}{12}h^3 f''(a) + \cdots$$

此即是公式 *(5.3),* 其誤差爲 $E = \frac{1}{12}h^3 f''(\xi)$. ■

Simpson's Rule

回憶梯形法 (the trapezoidal rule) 是以直線來近似$f(x)$(即線性函數近似法或稱爲一次多項式近似法). 若改以拋物線 (即二次多項式函數)來近似$f(x)$, 此種數值積分法稱爲 **Simpson's rule**. 茲敘述如下.

將$[a, b]$分割成 2 個等子區間 (即$x_0 = a, x_1 = (a+b)/2, x_2 = b$). 則在子區間 $[x_0, x_2]$ 有一二次多項式 (拋物線) 通過 $(x_0, f(x_0))$, $(x_1, f(x_1))$ 和 $(x_2, f(x_2))$ 三點, 設其方程式爲 $p(x) = Ax^2 + Bx + C$. Thus, the **Basic Simpson's Rule:** is

$$\int_{x_0}^{x_2} p(x)dx = \frac{x_2 - x_0}{6}[p(x_0) + 4p(x_1) + p(x_2)]$$

定理 **4.** *(二次函數之積分)* 若 $p(x) = Ax^2 + Bx + C$ 則

$$\int_a^b p(x)dx = \frac{b-a}{6}\left[p(a) + 4p\left(\frac{a+b}{2}\right) + p(b)\right]$$

PROOF:

$$\begin{aligned}
\int_a^b p(x)dx &= \int_a^b (Ax^2 + Bx + C)dx = \left[A\frac{x^3}{3} + B\frac{x^2}{2} + Cx\right]_a^b \\
&= \frac{A(b^3 - a^3)}{3} + \frac{B(b^2 - a^2)}{2} + C(b-a) \\
&= \frac{b-a}{6}[2A(a^2 + ab + b^2) + 3B(b+a) + 6C] \\
&= \frac{b-a}{6}\left\{(Aa^2 + Ba + C) + 4\left[A\left(\frac{b+a}{2}\right)^2 + B\left(\frac{b+a}{2}\right) + C\right] + (Ab^2 + Bb + C)\right\} \\
&= \frac{b-a}{6}\left[p(a) + 4p\left(\frac{a+b}{2}\right) + p(b)\right]
\end{aligned}$$

設函數f在$[a, b]$連續. 若將$[a, b]$分割成n等子區間 (let n be even), 即

$$P = \{x_0 = a < x_1 < x_2 < \ldots < x_n = b\}$$

則

$$h = \frac{b-a}{n}, \quad x_i = a + ih, \quad i = 1, 2, \ldots, n.$$

The composite Simposon's Rule is:

$$\int_a^b f(x)dx \approx \frac{h}{3}[f(x_0)+4f(x_1)+2f(x_2)+4f(x_3)+\cdots+4f(x_{n-1})+f(x_n)]$$

PROOF: 首先考慮

$$\begin{aligned}
\int_{x_0}^{x_2} f(x)dx &\approx \frac{x_2-x_0}{6}[f(x_0)+4f(x_1)+f(x_2)] = \frac{h}{3}[\cdots] \\
\int_{x_2}^{x_4} f(x)dx &\approx \frac{x_4-x_2}{6}[f(x_2)+4f(x_3)+f(x_4)] = \frac{h}{3}[\cdots] \\
\cdots & \cdots \cdots \\
\int_{x_{n-2}}^{x_n} f(x)dx &\approx \frac{x_n-x_{n-2}}{6}[f(x_{n-2})+4f(x_{n-1})+f(x_n)] = \frac{h}{3}[\cdots] \\
\int_a^b f(x)dx &= \sum_{i=1}^{n-1}\int_{x_{i-1}}^{x_{i+1}} f(x)dx \\
&\approx \frac{h}{3}[f(x_0)+4f(x_1)+2f(x_2)+\ldots+4f(x_{n-1})+f(x_n)] \\
\text{or } \int_a^b f(x)dx &\approx \frac{h}{3}\left[f(x_0)+4\sum_{k=1}^{n/2} f(x_{2k-1})+2\sum_{k=1}^{n/2-1} f(x_{2k})+f(x_n)\right]
\end{aligned}$$

Error Analysis for basic Simpson's Rule

首先證明

$$\int_a^{a+2h} f(x)dx \approx \frac{h}{3}[f(a)+4f(a+h)+f(a+2h)] \tag{5.11}$$

用 Taylor's Series 展開 $f(a+h)$ 和 $f(a+2h)$

$$f(a+h) = f(a)+hf'(a)+\frac{h^2}{2!}f''(a)+\frac{h^3}{3!}f'''(a)+\frac{h^4}{4!}f^{(4)}(a)+\cdots$$

將 $h \longleftarrow 2h$ 得

$$f(a+2h) = f(a)+2hf'(a)+\frac{(2h)^2}{2!}f''(a)+\frac{(2h)^3}{3!}f'''(a)+\frac{(2h)^4}{4!}f^{(4)}(a)+\cdots$$

將

$$\begin{aligned}
&\frac{h}{3}[f(a)+4f(a+h)+f(a+2h)] \\
&= 2hf+2h^2f'+\frac{4}{3}h^3f''+\frac{2}{3}h^4f'''+\frac{5}{18}h^{(5)}f^{(4)}+\cdots
\end{aligned} \tag{5.12}$$

設

$$F(x)=\int_a^x f(t)dt$$

則此積分

$$\begin{aligned}
&\int_a^{a+2h} f(x)dx = F(a+2h) \\
&= F(a)+2hF'(a)+2h^2F''(a)+\frac{4}{3}h^3F'''+\frac{2}{3}h^4F^{(4)}(a)+\frac{4}{15}h^5F^{(5)}(a)+\cdots
\end{aligned}$$

因 $F(a)=0,\ F'=f,\ F''=f',\ F'''=f''$, and so on. 故左式

$$\int_a^{a+2h} f(x)dx = 2hf+2h^2f'+\frac{4}{3}h^3f''+\frac{2}{3}h^4f'''+\frac{4}{15}h^5f^{(4)}+\cdots \tag{5.13}$$

由 (5.13) − (5.12) 得

$$\int_a^{a+2h} f(x)dx = \frac{h}{3}[f(a)+4f(a+h)+f(a+2h)]-\frac{h^5}{90}f^{(4)}+\cdots$$

因此, 由 Taylor's Theorem 知 the error term

$$E=-\frac{h^5}{90}f^{(4)}(\xi)=O(h^5) \quad \text{as } h\longrightarrow 0$$

其中 $\xi\in(a,\ a+2h)$. 因此有

定理 5. Basic Simpson's Rule

If $f\in C^4[a,\ b]$, then there exists a number ξ in $(a,\ b)$ with

$$\int_a^b f(x)dx=\frac{b-a}{6}\left[f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right]-\frac{f^{(4)}(\xi)}{2880}(b-a)^5. \tag{5.14}$$

Newton-Cotes Quadrature Rules

在實用上, 我們取區間 $[a, b]$ 的等分割 (uniform partition). 即 $\Delta x_i = h = (b-a)/n$ 且 $x_i = a + ih$, $0 \le i \le n$. 此種取等分區間之方法 (公式) 通稱爲 Newton-Cotes Rules. 我們已有

$$\begin{aligned} T(f;\, P) &= \frac{h}{2}\sum_{i=0}^{n-1}[f(x_i)+f(x_{i+1})] \\ &= h\left\{\sum_{i=1}^{n-1} f(x_i) + \frac{f(x_0)+f(x_n)}{2}\right\} \end{aligned} \tag{5.15}$$

定理 **6. Composite Midpoint Rule**

Suppose that $f \in C^2[a,b]$ *and* n *is even with* $h = \frac{b-a}{n+2}$ *and* $x_j = a + (j+1)h$*. Then there exists number* ξ *in* $(a,\, b)$ *such that*

$$\int_a^b f(x)\,dx = 2h\sum_{j=0}^{n/2} f(a+(2j+1)h) + \frac{(b-a)}{6}h^2 f''(\xi).$$

定理 **7. Composite Trapezoidal Rule**

Suppose that $f \in C^2[a,b]$*, Then there exists number* ξ *in* $(a,\, b)$ *such that*

$$\int_a^b f(x)\,dx = h\left[\frac{f(a)}{2} + \sum_{j=1}^{n-1} f(a+jh) + \frac{f(b)}{2}\right] - \frac{(b-a)}{12}h^2 f''(\xi). \tag{5.16}$$

定理 **8. Composite Simpson's Rule**

Suppose that $f \in C^4[a,\, b]$ *and* n *is even. Then there exists a number* ξ *in* $(a,\, b)$ *such that*

$$\int_a^b f(x)dx = \frac{h}{3}\left[f(a) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + 2\sum_{j=1}^{n/2-1} f(x_{2j}) + f(b)\right] - \frac{(b-a)}{180}h^4 f^{(4)}(\xi). \tag{5.17}$$

以上即我們實用上之 (合成) 辛普森法, (合成) 中點法, 和 (合成) 梯形法公式. 另有常用的 **Simpson's$\frac{3}{8}$ Rule**(4 points):

$$\int_{x_0}^{x_3} f(x)dx = \frac{3}{8}h\left[f(x_0)+3f(x_1)+3f(x_2)+f(x_3)\right] - \frac{3}{80}h^5 f^{(4)}(\xi). \tag{5.18}$$

and **Boole's Rule**(5 points):

$$\int_{x_0}^{x_4} f(x)dx = \frac{2}{45}h\left[7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4\right] - \frac{8}{945}h^7 f^{(6)}(\xi). \tag{5.19}$$

其梯形法程式如下表:

function int_sum = Trapezoid(f, a, b, n)
$h = (b-a)/n$
$int\_sum = \frac{1}{2}[f(a) + f(b)]$
for $i = 1$ **to** $n-1$ **do**,
  $x = a + ih$
  $int\_sum = int\_sum + f(x)$
end for
$int\_sum = int\_sum \times h$
end procedure

例題 **2.** *compute* $\int_0^1 \frac{\sin x}{x}dx$ *by using trapezoidal rule with 6 uniform points (n=5).*
解答*:*
取 P 為

$$P = \{x_0 = 0, x_1 = 0.2, x_2 = 0.4, x_3 = 0.6, x_4 = 0.8, x_5 = 1\}$$

則 $h = 1/5 = 0.2$ 且有

$$\begin{aligned} T(f;\, P) &= 0.2\left[\frac{f(0)}{2} + \sum_{i=1}^{4} f(x_i) + \frac{f(1)}{2}\right] \\ &= 0.94508 \end{aligned}$$

若應用Maple指令:
> $eval(Si(1));$ [Compute the $Si(x)$ function at $x = 1$.]
若應用Matlab指令:
> $quad8('f', 0, 1)$ [a recursive Newton-cotes 8 panel rule]

例題 **3.** *Use the composite trapezoidal rule to compute*

$$\int_0^1 e^{-x^2}dx$$

with an error at most $\frac{1}{2}\times 10^{-4}$. *How many points should be used? (*即求 $n=$?*)*

解答 :

By the error formula, $E=-\frac{b-a}{12}h^2 f''(\xi)$

例題 **4.** *Use the composite trapezoidal rule to approximate* $\int_0^1 \frac{\sin x}{x}dx$,
使其 *error* $\leq \frac{1}{2}\times 10^{-5}$, 問必須分割成多少個子區間*(*即求 $n=$*)?* 其中

$$f(x)=\begin{cases}\frac{\sin x}{x}, & x\neq 0\\ 1, & x=0\end{cases}$$

解答 :

欲求 $f''(x)$ 在 $[0,1]$ 之上界. 若以通常之導數則難以求其上界, 因 x 的正乘冪在分母, 故展開成其 *Taylor series*

$$\begin{aligned} f(x) &= \frac{\sin x}{x}=1-\frac{x^2}{3!}+\frac{x^4}{5!}-\frac{x^6}{7!}+\frac{x^8}{9!}-\ldots \\ f'(x) &= \frac{2x}{3!}+\frac{4x^3}{5!}-\frac{6x^5}{7!}+\frac{8x^7}{9!}-\ldots \\ f''(x) &= -\frac{2}{3!}+\frac{3\times 4x^2}{5!}-\frac{6\times 5x^4}{7!}+\frac{8\times 7x^6}{9!}-\ldots \end{aligned}$$

因 f 在 $[0,1]$ 區間, 故 $|f''(x)| \le \frac{1}{2}$ *because*

$$\begin{aligned} |f''(1)| &\le \frac{2}{3!} + \frac{3\times 4}{5!} + \frac{5\times 6}{7!} + \frac{7\times 8}{9!} + \cdots \\ &\le \frac{1}{3} + \frac{1}{10} + \frac{1}{24}(\frac{1}{2} + \frac{1}{4} + \frac{1}{8} + \ldots) < \frac{1}{2} \end{aligned}$$

故有

$$|\frac{b-a}{12}h^2 f''(\zeta)| \le \frac{h^2}{24} \le \frac{1}{2}\times 10^{-5} \quad 即 \frac{1}{24n^2} \le \frac{1}{2}\times 10^{-5}$$

解得 $n \ge 10^2/\sqrt{1.2} \approx 91.3$. 故至少取 $n = 92$ $\sharp$

5.3 Romberg Integration

Recursive Trapezoidal Formula for 2^n equal subintervals

The composite Trapezoidal rule is

$$\begin{aligned} T(f;\,P) &= h\left[\frac{f(x_0)}{2} + \sum_{i=1}^{n-1} f(x_i) + \frac{f(x_n)}{2}\right] \\ &= h\left[\frac{f(a)}{2} + \sum_{i=1}^{n-1} f(a+ih) + \frac{f(b)}{2}\right] \end{aligned}$$

這個公式是將 $[a, b]$ 分割成 n 個等子區間. 若改以分割成 2^n 個等子區間. 則 $h = (b-a)/2^n$ 且上面公式變成

$$R(n,0) = h\left[\frac{f(a)}{2} + \sum_{i=1}^{2^n-1} f(a+ih) + \frac{f(b)}{2}\right]$$

如此可應用於Romberg Algorithm

$$R(i,\,j) = R(i,j-1) + \frac{1}{4^j-1}[R(i,j-1) - R(i-1,j-1)], \quad i \ge 1,\, j \ge 1$$

and

$$R(i,0) = \frac{1}{2}R(i-1,0) + h\sum_{k=1}^{2^{i-1}} f(a+(2k-1)h)$$

應用此演算法在計算上可節省已算過之點, 並適用於任意精確度. 例如: $R(2,0)$ 即 $h=(b-a)/2^2$ 因在 $R(1,0)$ 已計算三個值 $f(a)$, $f(a+\frac{b-a}{2})$, $f(b)$. 故只要再算 $f\left(a+\frac{b-a}{4}\right)$ 和 $f\left(a+\frac{3(b-a)}{4}\right)$ 即可. 而在計算 $R(3,0)$ 時, 因 $R(2,0)$ 有5個點已計算. 只須再算4個點

$$f\left(a+\frac{(b-a)}{8}\right), f\left(a+\frac{3(b-a)}{8}\right), f\left(a+\frac{5(b-a)}{8}\right), \text{和 } f\left(a+\frac{7(b-a)}{8}\right)$$

因此, 我們有 recurrence relation:
若 $R(n-1,0)$ 已被 computed 且欲 compute $R(n,0)$:

$$\begin{aligned}R(n,0) &= \frac{1}{2}R(n-1,0)+\left[R(n,0)-\frac{1}{2}R(n-1,0)\right]\\ &= \frac{1}{2}R(n-1,0)+h\sum_{k=1}^{2^{n-1}} f(a+(2k-1)h)\end{aligned}$$

Fixing $h=(b-a)/2^n$ and putting

$$c=\frac{h}{2}[f(a)+f(b)]$$

we have

$$R(n,0) = h\sum_{i=1}^{2^n-1} f(a+ih)+c \tag{5.20}$$

$$R(n-1,0) = 2h\sum_{j=1}^{2^{n-1}-1} f(a+2jh)+2c \tag{5.21}$$

Notice: $R(n-1,0)$ 之子區間長度 h 是 $R(n,0)$ 之子區間長度<u>的兩倍</u>, 故乘以2

$$\begin{aligned}R(n,0)-\frac{1}{2}R(n-1,0) &= h\sum_{i=1}^{2^n-1} f(a+ih)-h\sum_{j=1}^{2^n-1} f(a+2jh)\\ &= h\sum_{k=1}^{2^{n-1}} f(a+(2k-1)h).\end{aligned}$$

To summarize:

定理 **9. Recursive Trapezoidal Formula**

若 $R(n-1,0)$ 是可用的, 則 $R(n,0)$ 可藉此公式

$$R(n,\,0)=\frac{1}{2}R(n-1,\,0)+h\sum_{k=1}^{2^{n-1}}f(a+(2k-1)h)$$

using $h=(b-a)/2^n$, where $R(0,0)=\frac{1}{2}(b-a)[f(a)-f(b)]$.

Romberg Algorithm

已分析得 trapezoidal rule 之一般精確度爲 $O(h^2)$, 即應用 Richardson extrapolation

$$I_h=\int_a^b f(x)\,dx=R(n-1,\,0)+a_2h^2+a_4h^4+a_6h^6+\cdots$$

其中 $h=(b-a)/2^{n-1}$.

$$\begin{aligned} I_{\frac{h}{2}}=\int_a^b f(x)dx &= R(n,0)+a_2\left(\frac{h}{2}\right)^2+a_4\left(\frac{h}{2}\right)^4+\cdots \\ &= R(n,0)+\frac{1}{4}a_2h^2+\frac{a_4}{16}h^4+\cdots \end{aligned}$$

定義：

$$R(n,\,1)=R(n,\,0)+\frac{1}{3}[R(n,0)-R(n-1,0)],\quad n\geq 1$$

則 $R(n,\,1)$ 的 accuracy 可達 $\underline{O(h^4)}$

如此繼續下去可求得

$R(n,2)$ 之 accuracy 爲 $O(h^6)$

$R(n,3)$ 之 accuracy 爲 $O(h^8)$

$\cdots\cdots\cdots$

$R(n,k)$ 之 accuracy 爲 $O(h^{2(k+1)})$

$R(n,n)$ 之 accuracy 爲 $O(h^{2(n+1)})$

因此 Romberg Algorithm 表成 <u>triangular array</u>

$$\left|\begin{array}{c} R(0,0) \\ R(1,0) \\ R(2,0) \\ \cdots \\ R(n,0) \end{array}\right| \begin{array}{c} \\ R(1,1) \\ R(2,1) \\ \cdots \\ R(n,1) \end{array} \Bigg| \begin{array}{c} \\ \\ R(2,2) \\ \cdots \\ R(n,2) \end{array} \Big| \begin{array}{c} \\ \\ \\ \cdots\cdots \\ \cdots\cdots \end{array} \Big| \begin{array}{c} \\ \\ \\ \\ R(n,n) \end{array} \Big|$$

$$\begin{aligned} R(0,0) &= \frac{1}{2}(b-a)[f(a)-f(b)] \\ R(1,0) &= \frac{1}{4}(b-a)\left[f(a)+f\left(\frac{a+b}{2}\right)\right]+\frac{b-a}{4}\left[f\left(\frac{a+b}{2}\right)+f(b)\right] \\ &= \frac{1}{4}(b-a)[f(a)+f(b)]+\frac{1}{2}(b-a)f\left(\frac{a+b}{2}\right) \\ &= \frac{1}{2}R(0,0)+\frac{1}{2}(b-a)f\left(\frac{a+b}{2}\right) \end{aligned}$$

因此程序繼續下去, 得

$$R(n,\,0)=\frac{1}{2}R(n-1,\,0)+h\sum_{k=1}^{2^{n-1}}f(a+(2k-1)h) \tag{5.22}$$

其中 $h=(b-a)/2^n$ and $n\geq 1$. 第2行和繼續下去之 columns in Romberg Array 可由 Richardson formula 得到

$$R(n,\,m)=R(n,\,m-1)+\frac{1}{4^m-1}[R(n,\,m-1)-R(n-1,\,m-1)] \tag{5.23}$$

其中 $n,\,m\geq 1$.

例題 **5.** 若 $R(4,2)=8$ 且 $R(3,2)=1$ 則 $R(4,3)=?$

解答:

$$\begin{aligned} R(4,3) &= R(4,2)+\frac{1}{3}[R(4,2)-R(3,2)] \\ &= \underline{8+\frac{1}{63}[8-1)=\frac{73}{9}}_{\sharp} \end{aligned}$$

Pseudocodes of the Romberg Algorithm

function $result$ = Romberg(f, a, b, n)
$R = zeros(n+1)$;   % Create a matrix $R(n+1, n+1)$.
$h = b - a$;
$R(0,0) = h * [f(a) + f(b)]/2$;
for i = 1 **to** n **do**
  $h = h/2$; $sum = 0$;
  % compute the first column $R(i, 0)$.
  for $k = 1$ **to** $2^i - 1$ **step** 2 **do**
    $x = a + k * h$;
    $sum = sum + f(x)$;
  end for
  $R(i,0) = R(i-1,0)/2 + sum * h$;

  for j = 1 **to** i **do**   % compute the $R(i, j)$, $j > 1$.
    $R(i, j+1) = R(i, j) + [R(i, j) - R(i-1, j)]/(4^j - 1)$;
  end for
end for
output $result = R(n+1, n+1)$
end function

5.4 An Adaptive Simpson's Rule

We have seen the **basic Simpson's rule**

$$\int_{x_0}^{x_2} p(x)dx = \frac{x_2 - x_0}{6}[p(x_0) + 4p(x_1) + p(x_2)]$$

and the **composite Simposon's rule**

$$\int_a^b f(x)dx \approx \frac{h}{3}[f(x_0)+4f(x_1)+2f(x_2)+4f(x_3)+\cdots+4f(x_{n-1})+f(x_n)].$$

The error of is Simpson's rule is $O(h^4)$. 但我們不知道 h 要多小才滿足我們所要求之精確度. 因此我們發展出自動選擇 h 之 Algorithm.

Adative Simpson's Algorithm

將 Simpson's rule 的應用一次寫成

$$I \equiv \int_a^b f(x)dx = S(a,\, b) + E(a,\, b)$$

其中

$$S(a,\, b) = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

$$E(a,\, b) = -\frac{1}{90}(\frac{b-a}{2})^5 f^{(4)}(\xi)$$

假定 $f^{(4)}(\xi) = \text{constant}$.
令 $h = b - a$ 以

$$I = S^{(1)} + E^{(1)} \tag{5.4}$$

$$S^{(1)} = S(a,\, b), \quad E^{(1)} = E(a,\, b) = -\frac{1}{90}\left(\frac{h}{2}\right)^5 f^{(4)}$$

應用 Simpson's rule 兩次 over $[a,\, b]$ 得

$$I = S^{(2)} + E^{(2)} \tag{5.5}$$

$$S^{(2)} = S(a, c) + S(c, b), \quad c = \frac{a+b}{2}$$

且

$$\begin{aligned} E^{(2)} &= -\frac{1}{90}\left(\frac{h/2}{2}\right)^5 f^{(4)} - \frac{1}{90}\left(\frac{h/2}{2}\right)^5 f^{(4)} = \frac{1}{16}E^{(1)} \\ \Rightarrow E^{(1)} &= 16E^{(2)} = \frac{1}{32}E^{(1)} + \frac{1}{32}E^{(1)} \end{aligned}$$

將 (5) − (4) 得

$$S^{(2)} - S^{(1)} = E^{(1)} - E^{(2)} = 16E^{(2)} - E^{(2)} = 15E^{(2)}$$

因此

$$I = S^{(2)} + E^{(2)} = S^{(2)} + \frac{1}{15}(S^{(2)} - S^{(1)})$$

故應用兩次的 Simpson's 法有 error

$$E^{(2)} = \frac{1}{15}|S^{(2)} - S^{(1)}| < \varepsilon \tag{5.6}$$

可用此公式當做所要精確度之規範 (the ciriterion of accuracy).

若 (6) 不滿足, 則將 $[a, b]$ 再分成兩個子區間 $[a, c]$ 和 $[c, b]$, $c = \frac{a+b}{2}$. 再要求這兩個子區間之積分, 使 (6) $< \frac{\varepsilon}{2}$. 則在 $[a, b]$ 時 $error < \frac{\varepsilon}{2} + \frac{\varepsilon}{2} = \varepsilon$. 令

$$I = \int_a^b f(x)dx = \int_a^c f(x)dx + \int_c^b f(x)dx = I_{left} + I_{right}$$

若 S 是 $S_{left}^{(2)}$ over $[a, c]$ 和 $S_{right}^{(2)}$ over $[c, b]$ 之和. 則有

$$\begin{aligned} |I - S| &= |I_{left} + I_{right} - S_{left}^{(2)} - S_{right}^{(2)}| \\ &\leq |I_{left} - S_{left}^{(2)}| + |I_{right} - S_{right}^{(2)}| \\ &= \frac{1}{15}|S_{left}^{(2)} - S_{left}^{(1)}| + \frac{1}{15}|S_{right}^{(2)} - S_{right}^{(1)}| \end{aligned}$$

若我們要求

$$\frac{1}{15}|I_l^{(2)} - S_l^{(1)}| < \frac{\varepsilon}{2}, \quad \frac{1}{15}|S_r^{(2)} - S_r^{(1)}| < \frac{\varepsilon}{2}$$

則 $|S - I| \leq \varepsilon$ 成立 over the entire interval $[a, b]$.

The pseudocode of the adative Simpson's algorithm

function $[result, level] = \text{adSimpson}(f, a, b, \varepsilon, level, level\_max)$
$level = level + 1$
$h = b - a$
$c = (a + b)/2$
$simpson1 = h[f(a) + 4f(c) + f(b)]/6$
$d = (a + c)/2$
$e = (b + c)/2$
$simpson2 = h[f(a) + 4f(d) + 2f(c) + 4f(e) + f(b)]/12$
if $level \geq level\_max$ **then**
  $result = simpson2$
  display "maximum level reached"
else
  if $|simpson2 - simpson1| < 15\varepsilon$ **then**
    $result = simpson2 + (simpson2 - simpson1)/15$
  else
    $left\_simpson = \text{adSimpson}(f, a, c, \varepsilon/2, level, level\_max)$
    $right\_simpson = \text{adSimpson}(f, c, b, \varepsilon/2, level, level\_max)$
    $result = left\_simpson + right\_simpson$
  end if
end if
end function

5.5 Gaussian Quadrature Rules

所有僅用函數值之數值積分法皆可表成如下型式:

$$\int_a^b f(x)dx \approx A_0 f(x_0) + A_1 f(x_1) + \cdots + A_n f(x_n)$$
$$= \sum_{i=0}^{n} A_i f(x_i) \qquad (5.7)$$

使用這種方法, 只須知道 the nodes $x_0, x_1, ..., x_n$ 和 the weights(權值或係數) $A_0, A_1, ..., A_n$.

例如, Trapezoidal and Simpson's rules 是取等距點 $x_i = a+ih$, $h = (b-a)/n$. $A_0 = A_n = 1/2$ and $A_i = 1, (i = 1, 2, \ldots, n-1)$ for Trapezoidal rule and $A_0 = A_n = 1$, $A_{2k-1} = 4, (k = 1, 2, \ldots, n/2)$ and $A_{2k} = 2, (k = 1, 2, \ldots, n/2 - 1)$ (letting n to be even) for Simpson's rules. 這種取等距點之方法通稱爲**Newton-Cotes rules**.

★ 另一種重要的特別方法是源自 interpolating polynomial $p(x)$ 近似 $f(x)$, 則 $\int_a^b p(x)dx$ 也必近似 $\int_a^b f(x)dx$ 的觀念來求其近似積分 (不論所給之 nodes 是否等距).

若 the nodes $x_0, x_1, ..., x_n$ 已知, 則存在一個對應的 Lagrange interpolation formula:

$$p(x) = \sum_{i=0}^{n} f(x_i)\ell_i(x) \text{ 其中 } \ell_i(x) = \prod_{\substack{j=0 \\ j\neq i}}^{n} \left(\frac{x - x_j}{x_i - x_j}\right) \quad (degree \leq n)$$

這個公式 (給我們) 提供一個次數 $\leq n$ 之多項式 $p(x)$, 其 interpolating 函數 f 在每一個 nodes, 即 $p(x_i) = f(x_i)$ for $0 \leq i \leq n$. 若在有利之情況, 則 p 是 f 的一個很好的近似函數, 且

$$\int_a^b p(x)dx \text{ 也是 } \int_a^b f(x)dx \text{ 的很好近似積分.}$$

因此,

$$\int_a^b f(x)dx \approx \int_a^b p(x)dx = \sum_{i=0}^{n} \int_a^b f(x_i)\ell_i(x)dx$$
$$= \sum_{i=0}^{n} A_i f(x_i) \qquad (5.8)$$

其中

$$A_i = \int_a^b \ell_i(x)dx. \tag{5.9}$$

由公式 (5.8) 被導出之方法中, 它將給每一次數$\leq n$ 之多項式的積分正確值.

例題 **1.** 決定一如型 *(5.7)* 之 *quadrature formula* 當 $x \in [-2, 2]$, 且 *the nodes are* $-1, 0, 1$.

解答*:*

(1) 先求出 $\ell_i(x)$*:*

(2) 再求 *weights* A_i*:* 由公式 *(2)*

因此*, the quadrature formula* 爲

$$\frac{8}{3}f(-1) - \frac{4}{3}f(0) + \frac{8}{3}f(1) \approx \int_{-2}^{2} f(x)dx.$$

以上公式對於任意次數小於或等於 *2* 之多項式, 均可給眞正值. 故可應用下列三函數來 *check* 這公式. 它給 $f(x) = 1$, x, *and* x^2 之積分眞正的值 *(exact* *values).*

Gaussian Nodes and Weights

由前面之討論, 理論上這些點 (nodes) 可任意給. 但事實上, 特別給的 nodes 能大大改進此數值積分之精確度(accuracy) 這由 Karl F. Gauss(1777-1885) 所發現, 稱爲 Gaussian quadrature.

定理 10. *(Gaussian quadrature Theorem)*
設 q 不爲 *0* 是次數 *n+1* 之多項式, 使得

$$\int_a^b x^k q(x)dx = 0 \quad (0 \le k \le n)$$

若 $x_0, x_1, ..., x_n$ 是 $q(x)$ 的 *zeros(*根*)*, 則

$$\int_a^b f(x)dx \approx \sum_{i=0}^{n} A_i f(x_i) \text{ 其中 } A_i = \int_a^b \ell_i(x)dx \tag{5.10}$$

用這些點 $x_i's$ 當 *nodes* 之以上公式, 將給所有的 *degree* $\le 2n+1$ 之多項式之積分眞正的值 *(exact values).* 其中 $\forall x_i \in (a,\, b)$.

證明 1. *(*只證第一 *assertion)*
設 f 是 *a polynomial of degree* $\le 2n+1$. *Divide* f *by* q, 得 *a quotient* p *and a remainder* r. 兩者之 *degree* $\le n$, 即

$$f = pq + r$$

由 *our hypothesis,* $\int_a^b q(x)p(x)dx = 0$ *(*因 p 的 *degree* $\le n$*)* 並且, 因每一個 x_i 是 q 的一個根, 我們有

$$f(x_i) = p(x_i)q(x_i) + r(x_i) = r(x_i) \quad \text{——} \quad (\star)$$

最後, 因 r 的 *degree* $\le n$, 公式 *(5.10)* 將給 $\int_a^b r(x)dx$ 精確的值*(precisely). Hence,*

$$\begin{aligned}\int_a^b f(x)dx &= \int_a^b p(x)q(x)dx + \int_a^b r(x)dx = \int_a^b r(x)dx \\ &= \sum_{i=0}^{n} A_i r(x_i) = \sum_{i=0}^{n} A_i f(x_i), \quad \text{由}(\star)\end{aligned}$$

結論:

(1) 若給任意 nodes, 公式 (5.10) 是 exact for all polynomials of *degree* $\le n$.

(2) 若給 Gaussian nodes (即 $g(x)$ 之根), 則公式 (5.10) 給 exact answers for all polynomials of *degree* $\le 2n+1$.

★ 由此定理之應用所得之 quadrature formulas(積分公式) 稱爲 Gaussian or Gauss-Legendre quadrature formulas. (The nodes are equivalent to the roots of the Legendre polynomials)

★ 對每一個區間 $[a, b]$ 和每一個 n, 存在一個不同之公式. 有更一般化的 Gaussian formulas 去近似如下之積分:

$$\int_0^\infty f(x)e^{-x}dx, \int_{-1}^1 f(x)(1-x^2)^{1/2}dx, \int_{-\infty}^\infty f(x)e^{-x^2}dx, \cdots, etc.$$

例題 **2.** 求以*3*個 *Gaussian nodes* 和*3*個 *weights* 試決定 $\int_{-1}^1 f(x)dx$ 的 *Gaussian quadrature formula.*

解答*:*

1. 必須找一 *polynomial* q *with degree=3* 且求其根. 設

$$q(x) = c_0 + c_1x + c_2x^2 + c_3x^3$$

則 q 必須滿足

$$\int_{-1}^1 q(x)dx = \int_{-1}^1 xq(x)dx = \int_{-1}^1 x^2q(x)dx = 0$$

Hence,

$$q(x) = 5x^3 - 3x$$

其 *roots* 爲 $-\sqrt{\frac{3}{5}}$, 0 和 $\sqrt{\frac{3}{5}}$, 這些即是*3-points Gaussian formula* 所要的 *nodes. 2.* 再求 *weights* A_0, A_1, 和 A_2, 應用未定係數法之 *procedure (the method of undetermined coefficients).* 欲求 A_0, A_1 和 A_2

$$\int_{-1}^{1} f(x)dx \approx A_0 f\left(-\sqrt{\frac{3}{5}}\right) + A_1 f(0) + A_2 f\left(\sqrt{\frac{3}{5}}\right). \tag{5.9}$$

只要 f 是二次多項式 $(ax^2 + bx + c)$, 則 " $\approx$ " *(approximate equality) becomes an* " $=$ " *exact equality.*
當然對 $f(x) = 1$, x, x^2 均成立. 因此

f	*Left-hand side*	*Right-hand side*
1	$\int_{-1}^{1} dx = 2$	$A_0 + A_1 + A_2 \Rightarrow A_0 + A_1 + A_2 = 2$
x	$\int_{-1}^{1} dx = 0$	$-\sqrt{\frac{3}{5}}A_0 + \sqrt{\frac{3}{5}}A_2 \Rightarrow A_0 = A_2$
x^2	$\int_{-1}^{1} x^2 dx = \frac{2}{3}$	$\frac{3}{5}A_0 + \frac{3}{5}A_2 \Rightarrow A_0 + A_2 = \frac{10}{9} \Rightarrow A_0 = A_2 = \frac{5}{9}$

$A_1 = \frac{8}{9}$ 因此最後之公式爲

$$\int_{-1}^{1} f(x)dx \approx \frac{5}{9} f\left(-\sqrt{\frac{3}{5}}\right) + \frac{8}{9} f(0) + \frac{5}{9} f\left(\sqrt{\frac{3}{5}}\right) \tag{5.10}$$

此積分將積所有 *degree* ≤ 5 次多項式 *(quintic polynomials) correctly.* 比如, $\int_{-1}^{1} x^4 dx = \frac{2}{5}$ 其右式也產生

$$\frac{2}{5} = \frac{5}{9}\left(-\sqrt{\frac{3}{5}}\right)^4 + \frac{8}{9}(0^4) + \frac{5}{9}\left(\sqrt{\frac{3}{5}}\right)^4.$$

若欲積 f 於 $[a, b]$. 則令 $t = [2x - (a+b)]/(b-a)$, 將 $[a, b]$ 之變換成在 $[-1, 1]$ 之積分, 應用一個 Gaussian quadrature rule

$$\int_{-1}^{1} f(t)dt \approx \sum_{i=0}^{n} A_i f(t_i)$$

$$\int_{a}^{b} f(x)dx = \frac{1}{2}(b-a)\int_{-1}^{1} f\left(\frac{1}{2}(b-a)t + \frac{1}{2}(b+a)\right) dt \tag{5.11}$$

區間之變換**:**

$$
\begin{aligned}
& t \in [0,1] \quad \xrightarrow{x=a+(b-a)t} \quad x \in [a,b] \quad \left(t = \frac{x-a}{b-a}\right) \\
& t \in [-1,1] \quad \xrightarrow{g(t)=f(a+(b-a)t)} \quad x \in [a,b] \\
& g(t) = f\left(\frac{1}{2}(b-a)t + \frac{1}{2}(b+a)\right) \quad \left(t = \frac{(x-a)+(x-b)}{b-a}\right).
\end{aligned}
$$

例題 **3.** 應用公式 *(5)* 和 *(6)* 去近似 $\int_0^1 e^{-x^2}dx$

解答 *:* 令 $a=0$, $b=1$

$$
\begin{aligned}
\int_0^1 f(x)dx &= \frac{1}{2}\int_{-1}^1 f\left(\frac{1}{2}t + \frac{1}{2}\right)dt \\
&= \frac{1}{2}\left[\frac{5}{9}f\left(-\frac{1}{2}\sqrt{\frac{3}{5}} + \frac{1}{2}\right) + \frac{8}{9}f\left(\frac{1}{2}\right) + \frac{5}{9}f\left(\frac{1}{2}\sqrt{\frac{3}{5}} + \frac{1}{2}\right)\right]
\end{aligned}
$$

放入 $f(x) = e^{-x^2}$ 得

$$
\begin{aligned}
\int_0^1 e^{-x^2}\,dx &\approx \frac{5}{18}e^{-0.112701665^2} + \frac{4}{9}e^{-0.5^2} + \frac{5}{18}e^{-0.887298335^2} \\
&\approx 0.746814584
\end{aligned}
$$

比較其眞值 $\frac{1}{2}\sqrt{\pi}\,erf(1) \approx 0.74682413281243$, 其誤差大約爲 10^{-5}. 故它是很好的近似值, 以只算 *3*個函數值而言.

結論: 很多多項式之根都可用來當 nodes, 如何用有效的方法去求這些多項式呢?

Legendre polynomial :

存在一些特殊多項式, 它的根可用來當 quadrature formulas 之 nodes. 例如: 將特殊化之積分 $\int_{-1}^1 f(x)dx$ 和標準化 $q_n(x)$ 使得 $q_n(1)=1$. 則這些多項式稱爲 Legendre polynomials. 用它的根來當 Gaussian quadrature 在區間 $[-1, 1]$ 的 nodes, 則只要再求出它對應的 weights A_i 即可. 前幾個 Legendre polynomials 爲:

$$\begin{aligned} q_0(x) &= 1 \\ q_1(x) &= x \\ q_2(x) &= \frac{3}{2}x^2 - \frac{1}{2} \\ q_3(x) &= \frac{5}{2}x^3 - \frac{3}{2}x \end{aligned}$$

它們可由一個三項式 recurrence relation 產生:

$$\begin{cases} q_n(x) = (\frac{2n-1}{n})x\, q_{n-1}(x) - \left(\frac{n-1}{n}\right) q_{n-2}(x), \quad n \geq 2 \quad \text{——} \quad (8) \\ q_0 = 1, \quad q_1 = x \end{cases}$$

它的 nodes 和 weights 已被建立成表. 其行成一系統化的積分公式 (Gaussian quadrature formulas): $\int_{-1}^{1} f(x)dx \approx \sum_{i=0}^{n} A_i f(x_i)$, 其他公式在 Abramowirtz and Stegun [1964] 之數學函數手册 (for n $\leq$ 95) 和 Stroud and Secrest(1966).

相同地觀念, 對於積分形如 $\int_a^b f(x)w(x)dx$ 其中 $w(x)$ 是固定的正函數, 定義於 $[a, b]$ 使得

$$\int_a^b x^n w(x)dx \ \text{均存在,} \ \forall n = 0, 1, 2, ...$$

一個重要的 $w(x)$ 的例子爲:

$$w(x) = \frac{1}{\sqrt{1-x^2}} \quad x \in [-1, 1].$$

其對應之定理爲:

定理 11. Weighted Gaussian Quadrature Theorem

若 q 是一非負, $degree = n + 1$ 之多項式, 使得

$$\int_a^b x^k q(x)w(x)dx = 0, \quad 0 \leq k \leq n$$

令 $x_0, x_1, ..., x_n$ 爲 q 的根, 則公式

$$\int_a^b f(x)w(x)dx \approx \sum_{i=0}^{n} A_i f(x_i) \quad \text{——} \quad (\star)$$

其中
$$A_i = \int_a^b \ell_i(x)w(x)dx \quad and \quad \ell_i(x) = \prod_{\substack{j=0\\j\neq i}}^{n} \frac{x-x_j}{x_i-x_j}.$$
此公式是 *exact* 當 f 是一個 *degree* $\le 2n+1$ 之多項式.
★ Gaussian formulas 有一很重要的優點: 是當一積分其函數在區間的一端是 infinite 時仍可適用.
即 $f(x)$ 允許其定義於 (a,b), $[a,b]$, and $(a,b]$, 且允許
$$\lim_{x\to a^+} f(x) = \pm\infty, \quad \lim_{x\to b^-} f(x) = \pm\infty.$$
因 Gaussian quadrature 永遠只用區間 $[a,\, b]$ 之內點 (interior points).

例題 **4.** 在計算 $\int_0^1 \frac{\sin x}{x}dx$ 可安全地使用 *Gaussian formulas* 因這些公式不會用到端點 $x=0$.
更複雜的例子*:*
$$\int_0^1 \frac{(x^2-1)^{1/3}}{\sqrt{\sin(e^x-1)}}dx$$
也可直接應用 *Gaussian formulas,* 儘管在 $x=0$ 是奇異點 *(singularity).* 或 $\int_0^1 1/\sqrt{x}dx$ 也一樣適用.

註: 求 Nodes 和 Weights 也有 elegant formulas 可自動計算出來, 可參考 Davis and Rabinowitz(1984) : "*Numerical Integration*" 或 Ghizetti and Ossiceini (1970).

結論: 一般積分公式有此型式
$$\int_a^b f(x)dx \approx \sum_{i=0}^{n} A_i f(x_i)$$
其中 A_i 是 weights. 此公式中, 若 the nodes are equally spaced(等距), 則稱爲 Nowton-Cotes formulas. 例如: the composite midpoint rule, the composite trapezoidal rule, the composite simpson's rule 都屬於 Nowton-Cotes formulas. 像例1之公式
$$\int_{-2}^{2} f(x)dx \approx \frac{8}{3}f(-1) - \frac{4}{3}f(0) + \frac{8}{3}f(1)$$

★ 也可用其他多項式之根當 nodes. 例如: Chebyshev polynomial 之根

$$x_i = \cos\left[\frac{(2i-1)\pi)}{2n}\right], \quad 1 \le i \le n$$