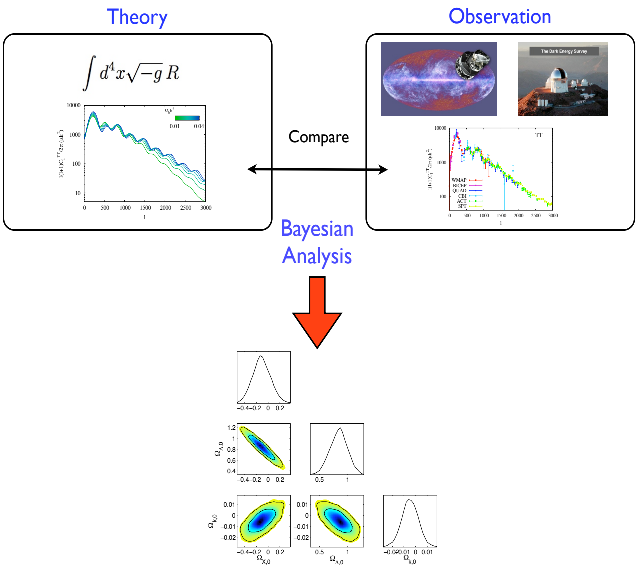
Numerical Methods



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In progress

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0.1 Numerical Differentiation and Integration

$$f'(x_0) = \frac{f(x_0+h) - f(x_0)}{h} - \frac{h}{2} f''(\xi)$$

This formula is known as the forward-difference formula if $h > 0$ and the backward-difference formula if $h < 0$. To obtain general derivative approximation formulas, suppose that $[x_0, x_1, \ldots, x_n]$ are $(n+1)$ distinct numbers in some interval I and that $f \in C^{n+1}(I)$. From Theorem (eq 67)

$$f(x) = \sum_{k=0}^{n} f(x_k) L_k(x) + \frac{(x-x_0)\cdots(x-x_n)}{(n+1)!} f^{(n+1)}(\xi(x)),$$

for some $\xi(x)$ in I, where $L_k(x)$ denotes the k-th Lagrange coefficient polynomial for f at $x_0, x_1, \ldots x_n$. Differentiating this expression gives (at x_j)

$$f'(x_j) = \sum_{k=0}^{n} f(x_k) L'_k(x_j) + \frac{f^{(n+1)}(\xi(x_j))}{(n+1)!} \Pi(x_j - x_k).$$

which is called an (n+1)-point formula to approximate $f'(x_j)$.

We first derive some useful three-point formulas. Since

$$L_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}, \quad \text{we have} \quad L'_0(x) = \frac{2x - x_1 - x_2}{(x_0-x_1)(x_0-x_2)}$$

Hence

$$\begin{aligned} f'(x_j) &= f(x_0)\left[\frac{2x_j - x_1 - x_2}{(x_0-x_1)(x_0-x_2)}\right] + f(x_1)\left[\frac{2x_j - x_0 - x_2}{(x_1-x_0)(x_1-x_2)}\right] \\ &+ f(x_2)\left[\frac{2x_j - x_0 - x_1}{(x_2-x_0)(x_2-x_1)}\right] + \frac{1}{6} f^{(3)}(\xi_j)\Pi^2(x_j - x_k), \end{aligned} \tag{1}$$

for each $j = 0, 1, 2$. Using with $x_j = x_0$, $x_1 = x_0 + h$ and $x_2 = x_0 + 2h$ gives

$$f'(x_0) = \frac{1}{h}\left[-\frac{3}{2} f(x_0) + 2f(x_1) - \frac{1}{2} f(x_2)\right] + \frac{h^2}{3} f^{(3)}(\xi_0)$$

Doing the same for $x_j = x_1$ and $x_j = x_2$

$$f'(x_1) = \frac{1}{h}\left[-\frac{1}{2} f(x_0) + \frac{1}{2} f(x_2)\right] + \frac{h^2}{6} f^{(3)}(\xi_1)$$

$$f'(x_2) = \frac{1}{h}\left[\frac{1}{2} f(x_0) - 2f(x_1) + \frac{3}{2} f(x_2)\right] + \frac{h^2}{3} f^{(3)}(\xi_2)$$

Since $x_1 = x_0 + h$ and $x_2 = x_0 + 2h$

and rewriting

$$f'(x_0) = \frac{1}{h}\left[-\frac{3}{2}f(x_0) + 2f(x_0+h) - \frac{1}{2}f(x_0+2h)\right] + \frac{h^2}{3}f^{(3)}(\xi_0).$$

$$f'(x_0+h) = \frac{1}{h}\left[-\frac{1}{2}f(x_0) + \frac{1}{2}f(x_0+2h)\right] - \frac{h^2}{6}f^{(3)}(\xi_1), \quad \text{and}$$

$$f'(x_0+2h) = \frac{1}{h}\left[\frac{1}{2}f(x_0) - 2f(x_0+h) + \frac{3}{2}f(x_0+2h)\right] + \frac{h^2}{3}f^{(3)}(\xi_2).$$

$$f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)] + \frac{h^2}{3}f^{(3)}(\xi_0),$$

$$f'(x_0) = \frac{1}{2h}[-f(x_0-h) + f(x_0+h)] - \frac{h^2}{6}f^{(3)}(\xi_1), \quad \text{and}$$

$$f'(x_0) = \frac{1}{2h}[f(x_0-2h) - 4f(x_0-h) + 3f(x_0)] + \frac{h^2}{3}f^{(3)}(\xi_2).$$

The last of these equations can be obtained from the first by replacing h with $-h$. Although errors are $\mathcal{O}(h^2)$, the middle is approximately half, because uses both sides of x_0.

Similarly there are five-point formulas whose error term is $\mathcal{O}(h^4)$

$$f'(x_0) = \frac{1}{12h}[f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)] + \frac{h^4}{30}f^{(5)}(\xi),$$

$$f'(x_0) = \frac{1}{12h}[-25f(x_0) + 48f(x_0+h) - 36f(x_0+2h)$$
$$+ 16f(x_0+3h) - 3f(x_0+4h)] + \frac{h^4}{5}f^{(5)}(\xi),$$

(hw: $f'(x) = (x+1)e^x$ and error, in range:[1.8, 2.2, 0.1], using three-point f/b: h=0.1, -0.1, middle: h=0.1, 0.2. middle five point: h=0.1)

$$f''(x_0) = \frac{1}{h^2}[f(x_0 - h) - 2f(x_0) + f(x_0 + h)] - \frac{h^2}{12}f^{(4)(\xi)}$$

0.2 Numerical integration

The basic method involved in approximating $\int_a^b f(x)dx$ is called numerical quadrature. It uses a sum

$$\sum_{i=0}^{n} a_i f(x_i)$$

to approximate $\int_a^b f(x)dx$. The methods of quadrature are based on the interpolation polynomials. We integrate the Lagrange interpolating polynomial

$$P_n(x) = \sum_{i=0}^{n} f(x_i)L_i(x)$$

and its truncation error term over $[a, b]$ to obtain

$$\int_a^b f(x)\,dx = \int_a^b \sum_{i=0}^{n} f(x_i)L_i(x)\,dx + \int_a^b \prod_{i=0}^{n}(x - x_i)\frac{f^{(n+1)}(\xi(x))}{(n+1)!}\,dx$$
$$= \sum_{i=0}^{n} a_i f(x_i) + \frac{1}{(n+1)!}\int_a^b \prod_{i=0}^{n}(x - x_i) f^{(n+1)}(\xi(x))\,dx,$$

where $\xi(x)$ is in $[a, b]$ for each x and

$$a_i = \int_a^b L_i(x)dx \quad \text{for each } i = 0, 1, ...n$$

The quadrature formula is therefore

$$\int_a^b f(x)dx \approx \sum_{i=0}^{n} a_i f(x_i)$$

0.3 Trapezoidal rule

Let $x_0 = a, x_1 = b$, $h = b - a$ and use the linear Lagrange polynomial:

$$P_1(x) = \frac{x - x_1}{x_0 - x_1}f(x_0) + \frac{x - x_0}{x_1 - x_0}f(x_1)$$

Then

$$\int_a^b f(x)dx = \int_{x_0}^{x_1} \left[\frac{x-x_1}{x_0-x_1} f(x_0) + \frac{x-x_0}{x_1-x_0} f(x_1) \right] dx - \frac{h^3}{12} f''(\xi)$$

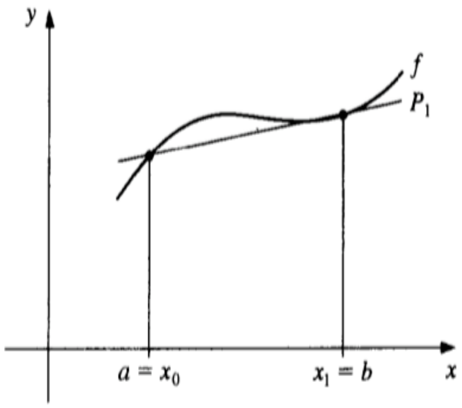
Consequently

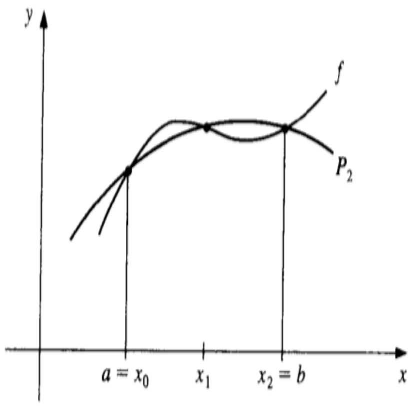
$$\int_a^b f(x)dx = \int_{x_0}^{x_1} \left[\frac{(x-x_1)^2}{2(x_0-x_1)} f(x_0) + \frac{(x-x_0)^2}{2(x_1-x_0)} f(x_1) \right] dx - \frac{h^3}{12} f''(\xi) \quad (2)$$

$$= \frac{x_1-x_0}{2}[f(x_0)+f(x_1)] - \frac{h^3}{12} f''(\xi) \quad (3)$$

and therefore

$$\int_a^b f(x)dx = \frac{h}{2}[f(x_0)+f(x_1)] - \frac{h^3}{12} f''(\xi) \quad (4)$$





0.4 Simpson's rule

Results from integrating over $[a, b]$ the second Lagrange polynomial with nodes $x_0 = a, x_2 = b$ and $x_1 = a + h$, where $h = (b - a)/2$, or an alternative formula. Suppose that f is expanded in the third Taylor polynomial about x_1. Then for each x in $[x0, x2]$

$$f(x) = f(x_1) + f'(x_1) + \frac{f''(x_1)}{2}(x-x_1)^2 + \frac{f'''(x_1)}{6}(x-x_1)^3 + \frac{f^{(4)}(\xi(x))}{24}(x-x_1)^4 \quad (5)$$

$$\int_{x_0}^{x_2} f(x)dx = \left[f(x_1)(x-x_1) + \frac{f'(x_1)}{2}(x-x_1)^2 + \frac{f''(x_1)}{6}(x-x_1)^3 + \frac{f'''(x_1)}{24}(x-x_1)^4 \right]_{x1}^{x_2} + O(h^5)$$

However $h = x_2 - x_1 = x_1 - x + 0$. Consequently

$$\int_{x_0}^{x_2} f(x)dx = 2hf(x_1) + \frac{h^3}{3}f''(x_1) + O(h^5)$$

If we now replace $f''(x_1)$ by the approximation, we have

$$\int_{x_0}^{x_2} f(x)dx = 2hf(x_1) + \frac{h^3}{3}\left\{\frac{1}{h^2}\left[f(x_0) - 2f(x_1) + f(x_2) + O(h^2)\right]\right\} + O(h^5)$$

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right] + O(\frac{h^5}{90})$$

0.5 closed Newton- Cotes

$n = 1$**: Trapezoidal rule**

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}[f(x_0) + f(x_1)] - \frac{h^3}{12}f''(\xi) \tag{6}$$

$n = 2$**: Simpson's rule**

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right] + \frac{h^5}{90}f^{(4)}(\xi) \tag{7}$$

$n = 3$**: Simpson's 3/8 rule**

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

$n = 4$**:**

$$\int_{x_0}^{x_4} f(x)dx = \frac{2h}{45}\left[7f(x_0) + 32f(x_1) + 12f(x_2) + 32f(x_3) + 7f(x_4)\right] - \frac{8h^7}{945}f^{(6)}(\xi) \tag{9}$$

0.6 open Newton- Cotes

$n = 0$**: Midpoint rule**

$$\int_{x_{-1}}^{x_1} f(x)dx = 2hf(x_0) + \frac{h^3}{3}f''(\xi) \tag{10}$$

$n = 1$**:**

$$\int_{x_{-1}}^{x_2} f(x)dx = \frac{3h}{2}\left[f(x_0) + f(x_1)\right] + \frac{3h^3}{4}f''(\xi) \tag{11}$$

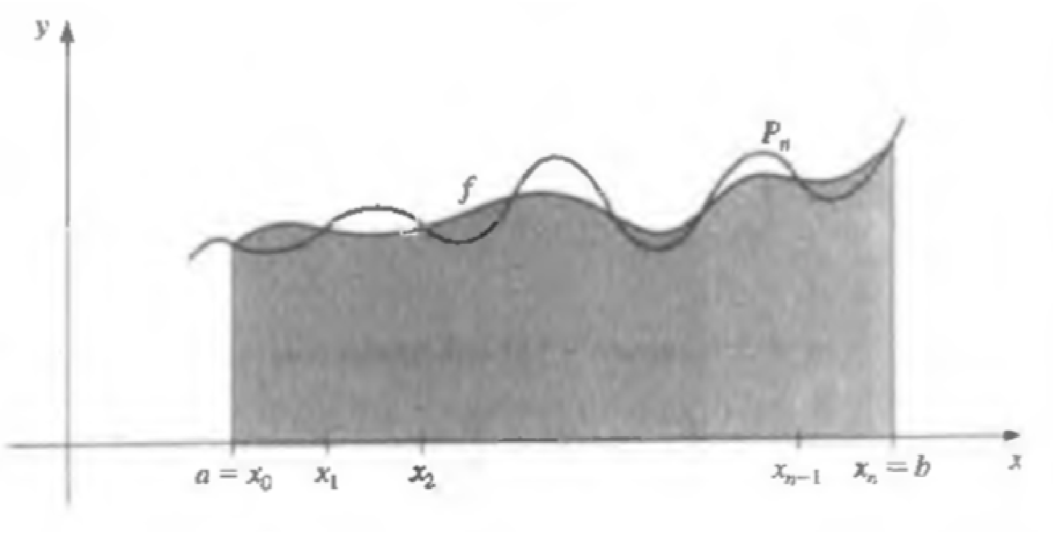
Suppose that $\sum_{i=0}^{n} a_i f(x_i)$ denotes the $(n+1)$-point closed Newton-Cotes formula with $x_0 = a$, $x_n = b$, and $h = (b-a)/n$. There exists $\xi \in (a, b)$ for which

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_0^n t^2(t-1)\cdots(t-n)\,dt,$$

if n is even and $f \in C^{n+2}[a, b]$, and

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_0^n t(t-1)\cdots(t-n)\,dt,$$

if n is odd and $f \in C^{n+1}[a, b]$. ∎



$n = 2$:

$$\int_{x_{-1}}^{x_3} f(x)dx = \frac{4h}{3}\left[2f(x_0) - f(x_1) + 2f(x_2)\right] + \frac{14h^5}{45} f^{(4)}(\xi) \tag{12}$$

$n = 3$:

$$\int_{x_{-1}}^{x_4} f(x)dx = \frac{5h}{24}\left[11f(x_0) + f(x_1) + f(x_2) + 11f(x_3)\right] + \frac{95h^5}{144} f^{(4)}(\xi) \tag{13}$$

(hw: $f(x)[0,2]$, $x^2, x^4, 1/(1+x), \sqrt{1+x^2}, \sin x, e^x$, Trapezoidal, Simpsons, Simpsons 3/8)

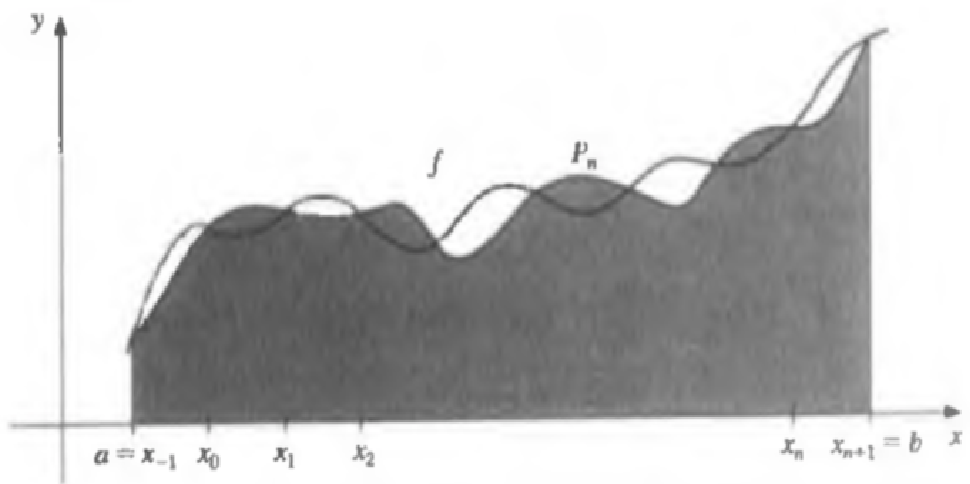
Suppose that $\sum_{i=0}^{n} a_i f(x_i)$ denotes the $(n+1)$-point open Newton-Cotes formula with $x_{-1} = a$, $x_{n+1} = b$, and $h = (b-a)/(n+2)$. There exists $\xi \in (a,b)$ for which

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_{-1}^{n+1} t^2(t-1)\cdots(t-n)\,dt,$$

if n is even and $f \in C^{n+2}[a,b]$, and

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_{-1}^{n+1} t(t-1)\cdots(t-n)\,dt,$$

if n is odd and $f \in C^{n+1}[a,b]$. ■



(hw: $\int_0^2 e^{2x} \sin 3x dx$, $n = ?$, h, Midpoint, Trapezoidal, Simpson, 10^{-4})

Let $f \in C^2[a,b]$, n be even, $h = (b-a)/(n+2)$, and $x_j = a + (j+1)h$ for each $j = -1, 0, \ldots, n+1$. There exists a $\mu \in (a,b)$ for which the **Composite Midpoint rule** for $n+2$ subintervals can be written with its error term as

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

Let $f \in C^2[a,b]$, $h = (b-a)/n$, and $x_j = a + jh$, for each $j = 0, 1, \ldots, n$. There exists a $\mu \in (a,b)$ for which the **Composite Trapezoidal rule** for n subintervals can be written with its error term as

$$\int_a^b f(x)\,dx = \frac{h}{2}\left[f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right] - \frac{b-a}{12}h^2 f''(\mu). \qquad \blacksquare$$

Let $f \in C^4[a,b]$, n be even, $h = (b-a)/n$, and $x_j = a + jh$, for each $j = 0, 1, \ldots, n$. There exists a $\mu \in (a,b)$ for which the **Composite Simpson's rule** for n subintervals can be written with its error term as

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

$\blacksquare$

0.7 Composite Numerical Integration

0.8 Unequal Segments

0.9 Romberg integration

Richardson's extrapolation, are error-correction techniques use two estimates of an integral to compute a third, more accurate approximation.

$$\int_a^b f(x)dx = \frac{h}{2}\left[f(a) + f(b) + 2\sum_{j=1}^{m-1} f(x_j)\right] - h^2 K_2 \tag{14}$$

$x_j = a + jh$. We use $m_1 = 1, m_2 = 2, m_3 = 4$, and $m_n = 2^{n-1}$. The step size corresponding to m_k is $h_k = (b-a)/m_k = (b-a)/2^{k-1}$. Then,

$$\int_a^b f(x)dx = \frac{h_k}{2}\left[f(a) + f(b) + 2\left(\sum_{i=1}^{2^{k-1}-1} f(a + ih_k)\right)\right] - h^2 K_2 \tag{15}$$

The parenthesis, we call it R_{k_l}, to then

$$R_{1,1} = \frac{h_1}{2}[f(a) + f(b)] = \frac{(b-a)}{2}[f(a) - f(b)] \tag{16}$$

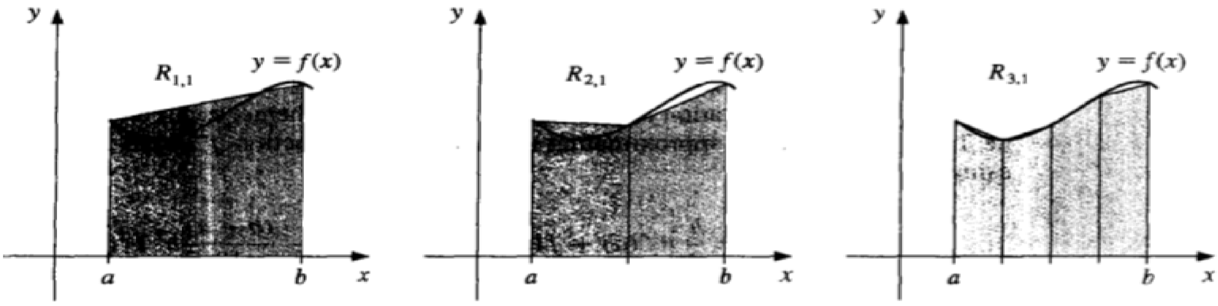
$$\begin{aligned} R_{2,1} &= \frac{h_2}{2}[f(a) + f(b) + 2f(a + h_2)] &(17)\\ &= \frac{(b-a)}{4}\left[f(a) + f(b) + 2f\left(a + \frac{(b-a)}{2}\right)\right] &(18)\\ &= \frac{1}{2}[R_{1,1} + h_1 f(a + h_2)] &(19)\end{aligned}$$

$$R_{k,1} = \frac{1}{2}\left[R_{k-1,1} + h_{k-1}\sum_{i=1}^{2^{k-2}} f(a + (2i-1)h_k)\right] \tag{20}$$

(py: do it)

0.10 Richardon's extrapolation

Suppose that we have a formula $N(h)$ that approximates a unknown value M and the truncation error has the form



$$M = N(h) + K_1 h + K_2 h^2 + K_3 h^3 \dots$$

Consider the result when we replace the parameter h by half its value. Then

$$M = N\left(\frac{h}{2}\right) + K_1 \frac{h}{2} + K_2 \frac{h}{4}^2 + K_3 \frac{h}{8}^3 \dots$$

Substracting them ($\times 2$)

$$M = \left[N\left(\frac{h}{2}\right) + \left(N\left(\frac{h}{2}\right) - N(h)\right)\right] + K_2\left(\frac{h^2}{2} - h^2\right) + K_3\left(\frac{h^3}{4} - h^3\right) \tag{21}$$

We define

$$N_2(h) = N_1\left(\frac{h}{2}\right) + \left[N_1\left(\frac{h}{2}\right) - N_1(h)\right]$$

Therefore, we have the $\mathcal{O}(h^2)$

$$M = N_2(h) - \frac{K_2}{2} h^2 - \frac{3K_3}{4} h^3 - \cdots$$

If we replace h by $h/2$ in this formula we have

$$M = N_2\left(\frac{h}{2}\right) - \frac{K_2}{8} h^2$$

and after some algebra, we have

$$M = N_3(h) + \frac{K_3}{8} h^3$$

In gral

$$M = N(h) + \sum_{j=1}^{m-1} K_j h^j + \mathcal{O}(h^m)$$

then for each $j = 2, 3, ..., m$

$$N_j(h) = N_{j-1}\left(\frac{h}{2}\right) + \frac{N_{j-1}(h/2) - N_{j-1}(h)}{2^{j-1} - 1}$$

Applied to Trapezoidal formula, with $k = 2, 3, \ldots, n$

$$R_{k,j} = R_{k,j-1} + \frac{R_{k,j-1} - R_{k-1,j-1}}{4^{j-1} - 1}$$

$R_{1,1}$					
$R_{2,1}$	$R_{2,2}$				
$R_{3,1}$	$R_{3,2}$	$R_{3,3}$			
$R_{4,1}$	$R_{4,2}$	$R_{4,3}$	$R_{4,4}$		
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	
$R_{n,1}$	$R_{n,2}$	$R_{n,3}$	$R_{n,4}$	$\cdots$	$R_{n,n}$

0.11 Adaptative Quadrature Methods

Adaptive quadrature methods adjust the step size so that small intervals are used in regions of rapid variations and larger intervals are used where the function changes gradually.

Apply Simpson's with step size $h = (b - a)/2$

$$\int_a^b f(x)dx = S(a,b) - \frac{h^5}{90} f^{(4)}(\mu)$$

where

$$S(a,b) = \frac{h}{3}[f(a) + 4f(a+h) + f(b)]$$

Now, we apply the Composite Simpson's rule with $n = 4$ and step size $(b - a)/4 = h/2$

$$\int_a^b f(x)dx = \frac{h}{6}\left[f(a) + 4f\left(a + \frac{h}{2}\right) + 2f(a+h) + 4f\left(a + \frac{3h}{2}\right) + f(b)\right] - \left(\frac{h}{2}\right)^4 \frac{(b-a)}{180} f^{(4)}(\mu)$$

To simplify notation

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

and

$$S\left(\frac{a+b}{2}, b\right) = \frac{h}{6}\left[f(a+h) + 4f\left(a + \frac{3h}{2}\right) + f(b)\right].$$

$$\int_a^b f(x)\,dx = S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, b\right) - \frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\tilde{\mu}).$$

$$S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, a\right) - \frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\mu) \approx S(a,b) - \frac{h^5}{90} f^{(4)}(\mu) \tag{22}$$

so

$$\frac{h^5}{90} f^{(4)}(\mu) \approx \frac{16}{15}\left[S(a,b) - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, a\right)\right] \tag{23}$$

$$\left|\int_a^b f(x)\,dx - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right| \approx \frac{1}{15}\left|S(a,b) - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right|.$$

Thus if,

When the approximation differ by more than 15ϵ, we apply the Simpson's rule technique individually to the subintervals $[a, (a+b)/2]$ and $[(a+b)/2, b]$. Then we use the error estimation procedure to determine if the approximation to the integral on each subinterval is within a tolerance of $\epsilon/2$. If so, we sum the approximations.

(hw: integral in first hw, w/ Exact, Trapez, Sim, Quad)

$$\left| S(a,b) - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right) \right| < 15\varepsilon,$$

we expect to have

$$\left| \int_a^b f(x)\,dx - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right) \right| < \varepsilon,$$

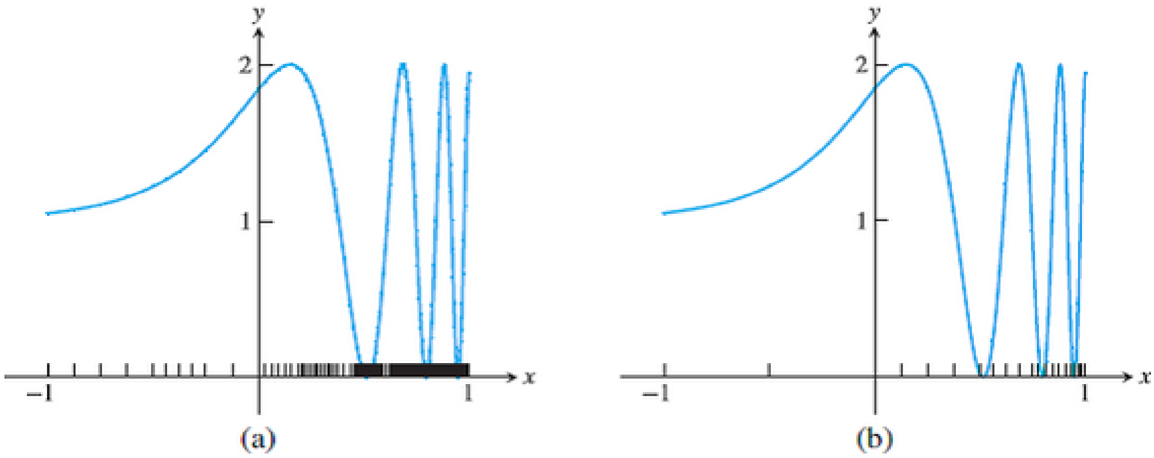


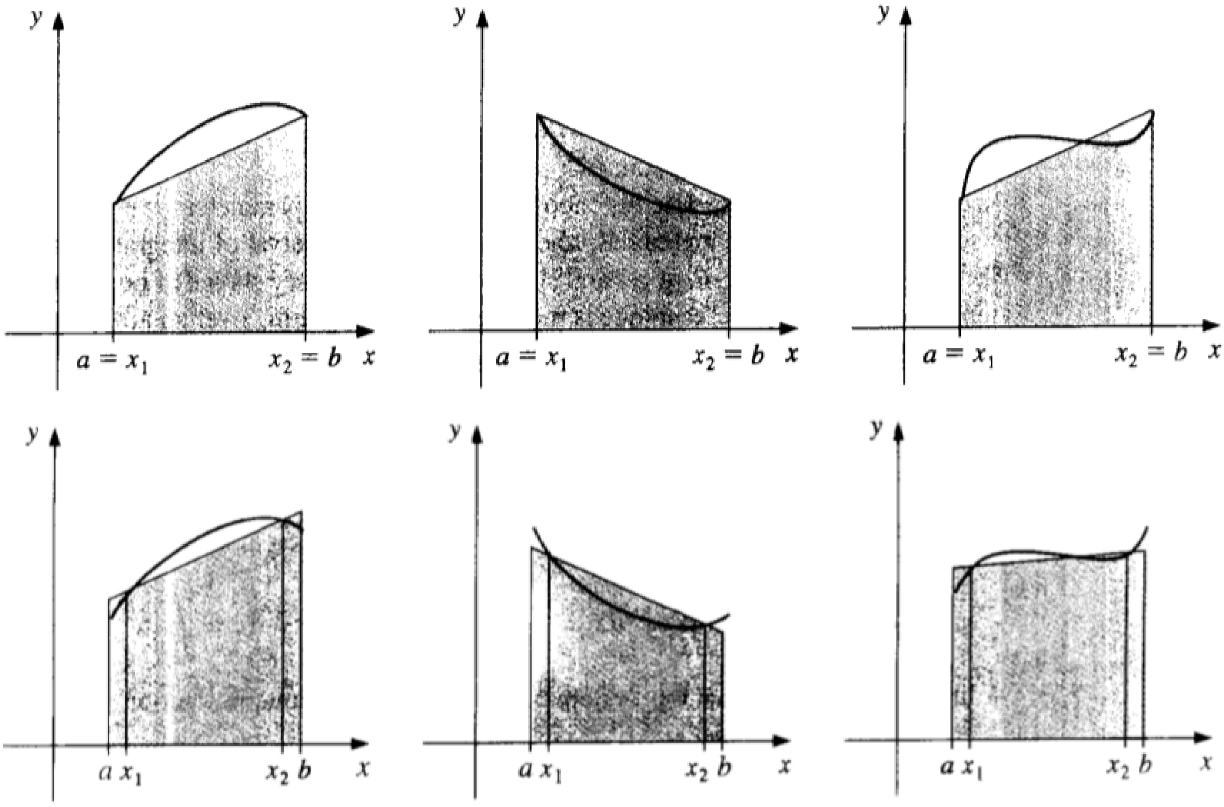
Figure 5.5 Adaptive quadrature applied to $f(x) = 1 + \sin e^{3x}$. Tolerance is set to TOL = 0.005. (a) Adaptive Trapezoid Rule requires 140 subintervals. (b) Adaptive Simpson's Rule requires 20 subintervals.

0.12 Multiple Integrals

(py: github)

0.13 Gaussian Quadrature

All the Newton-Cotes formulas use values of the function at equally-spaced points. Gaussian quadrature chooses the points for evaluation in an optimal, rather than equally spaced way. This restriction is convenient when the formulas are combined to form the composite rules, but it can significantly decrease the accuracy of the approximation.



Gaussian quadrature chooses the points for evaluation in an optimal, rather than equally spaced, way. The nodes $x_1, x_2, ...x_n$ in the interval $[a, b]$ and coefficients $c_1, c_2, ...c_n$ are chosen to minimize the expected error obtained in the approximation

$$\int_a^b f(x)dx \approx \sum_{i=1}^{n} c_i f(x_i)$$

For illustration, we select the coefficients and nodes when $n = 2$ and the interval of integration is $[-1, 1]$.

Suppose we want to determine c_1, c_2, x_1 and x_2

$$\int_{-1}^{1} f(x)dx \approx c_1 f(x_1) + c_2 f(x_2)$$

gives the exact result whenever $f(x)$ is a polynomial of degree 3 or less, that is, when

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3$$

with a little of algebra

$$c_1 = 1, \quad c_2 = 1, \quad x_1 = -\frac{\sqrt{3}}{3} \quad x_2 = \frac{\sqrt{3}}{3}$$

which gives the approximation formula

$$\int_{-1}^{1} f(x)dx \approx f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right)$$

This technique could be used to determine the nodes and coefficients for formulas that give exact results for higher-degree polynomials.

1. For each n, $P_n(x)$ is a polynomial of degree n.
2. $\int_{-1}^{1} P(x)P_n(x)\,dx = 0$ whenever $P(x)$ is a polynomial of degree less than n.

The first few Legendre polynomials are

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

$$P_3(x) = x^3 - \frac{3}{5}x, \quad \text{and} \quad P_4(x) = x^4 - \frac{6}{7}x^2 + \frac{3}{35}.$$

An integral $\int_a^b f(x)dx$ over an arbitrary $[a, b]$ can be transformed into an integral over $[-1, 1]$ by using the change of variables

$$t = \frac{2x - a - b}{b - a} \to x = \frac{1}{2}[(b - a)t + a + b]$$

This permits Gaussian quadrature to be applied to any interval $[a, b]$, since

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

(hw: $\int_0^{\pi/4} x^2 \sin x dx$, $\int_0^1 x^2 e^{-x} dx$, n=3,4. Romberg n=4)

Suppose that $x_1, x_2, \ldots, x_n$ are the roots of the nth Legendre polynomial $P_n(x)$ and that for each $i = 1, 2, \ldots, n$, the numbers c_i are defined by

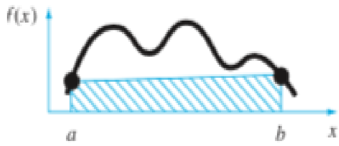
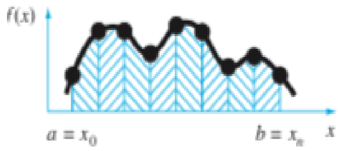
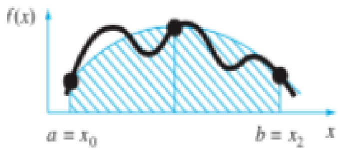
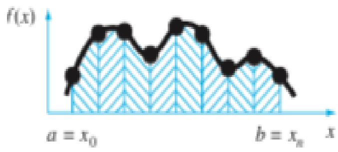
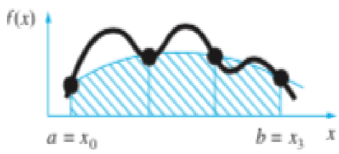
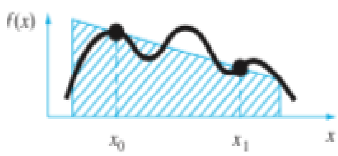
$$c_i = \int_{-1}^{1} \prod_{\substack{j=1 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}\, dx.$$

If $P(x)$ is any polynomial of degree less than $2n$, then

$$\int_{-1}^{1} P(x)\, dx = \sum_{i=1}^{n} c_i P(x_i). \qquad \blacksquare$$

n	Roots $r_{n,i}$	Coefficients $c_{n,i}$
2	0.5773502692	1.0000000000
	−0.5773502692	1.0000000000
3	0.7745966692	0.5555555556
	0.0000000000	0.8888888889
	−0.7745966692	0.5555555556
4	0.8611363116	0.3478548451
	0.3399810436	0.6521451549
	−0.3399810436	0.6521451549
	−0.8611363116	0.3478548451
5	0.9061798459	0.2369268850
	0.5384693101	0.4786286705
	0.0000000000	0.5688888889
	−0.5384693101	0.4786286705
	−0.9061798459	0.2369268850

Method	Data Points Required for One Application	Data Points Required for n Applications	Truncation Error	Application	Programming Effort	Comments
Trapezoidal rule	2	$n+1$	$\simeq h^3 f''(\xi)$	Wide	Easy	
Simpson's 1/3 rule	3	$2n+1$	$\simeq h^5 f^{(4)}(\xi)$	Wide	Easy	
Simpson's rule (1/3 and 3/8)	3 or 4	≥ 3	$\simeq h^5 f^{(4)}(\xi)$	Wide	Easy	
Higher-order Newton-Cotes	≥ 5	N/A	$\simeq h^7 f^{(6)}(\xi)$	Rare	Easy	
Romberg integration	3			Requires $f(x)$ be known	Moderate	Inappropriate for tabular data
Gauss quadrature	≥ 2	N/A		Requires $f(x)$ be known	Easy	Inappropriate for tabular data

Method	Formulation	Graphic Interpretations	Error
Trapezoidal rule	$I = (b-a)\dfrac{f(a)+f(b)}{2}$		$-\dfrac{(b-a)^3}{12} f''(\xi)$
Multiple-application trapezoidal rule	$I = (b-a)\dfrac{f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)}{2n}$		$-\dfrac{(b-a)^3}{12n^2}\bar{f}''$
Simpson's 1/3 rule	$I = (b-a)\dfrac{f(x_0)+4f(x_1)+f(x_2)}{6}$		$-\dfrac{(b-a)^5}{2880} f^{(4)}(\xi)$
Multiple-application Simpson's 1/3 rule	$I = (b-a)\dfrac{f(x_0) + 4\sum_{i=1,3}^{n-1} f(x_i) + 2\sum_{j=2,4}^{n-2} f(x_j) + f(x_n)}{3n}$		$-\dfrac{(b-a)^5}{180n^4}\bar{f}^{(4)}$
Simpson's 3/8 rule	$I = (b-a)\dfrac{f(x_0)+3f(x_1)+3f(x_2)+f(x_3)}{8}$		$-\dfrac{(b-a)^5}{6480} f^{(4)}(\xi)$
Romberg integration	$I_{j,k} = \dfrac{4^{k-1} I_{j+1,k-1} - I_{j,k-1}}{4^{k-1}-1}$		$O(h^{2k})$
Gauss quadrature	$I = c_0 f(x_0) + c_1 f(x_1) + \cdots + c_{n-1} f(x_{n-1})$		$\simeq f^{(2n+2)}(\xi)$