CHAPTER 10

Numerical Integration

Introduction

- Many definite integrals of interest can't be evaluated analytically.
- Probably the best-known example is the integral that gives the area under the standard bell-shaped curve, given by

$$F(x) = \frac{1}{2} + \frac{1}{\sqrt{2\pi}} \int_0^x e^{-z^2/2} dz$$

- This integral appears very frequently in probability and statistics and is extensively tabulated.

- The integral is tabulated because it is a fact that there is no way to express the anti-derivative of $\exp(-z^2)$ in terms of elementary functions.
- Because of cases like this, we need methods to perform approximate integration; for other cases it may be more convenient to use a numerical method than a symbolic one.
- Often we're given values of $f(x)$ at various points but not a formula for f and so have no choice but to use a numerical method (for example, data from an experiment).

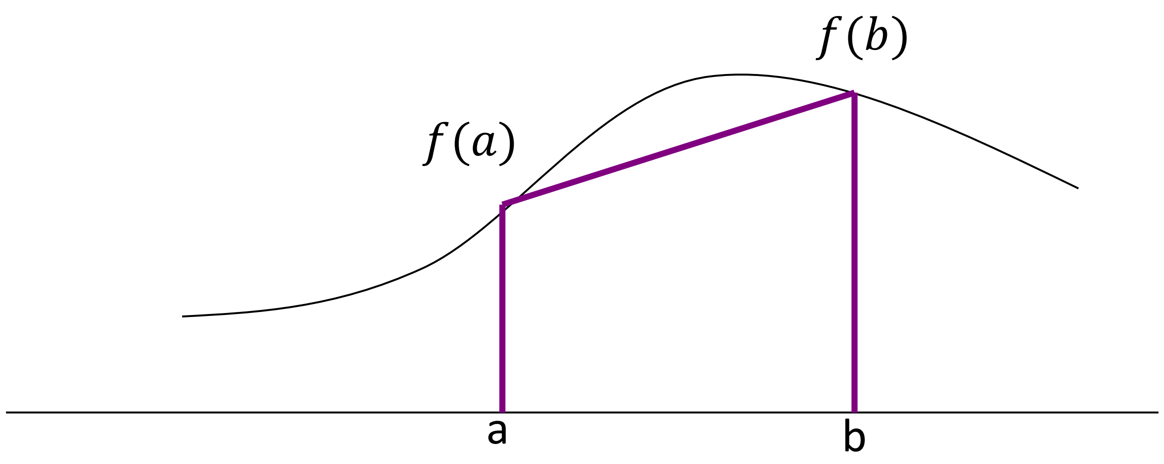
Formula

- The Newton-Cotes formula:
  - Trapezoidal Rule
  - Simpson's Rule

- Romberg Integration

Trapezoidal Rule

- The trapezoidal rule is equivalent to approximating the area of the trapezoid under the straight line connecting $f(a)$ and $f(b)$.



- One way to improve the accuracy of the trapezoid rule is to divide the integration interval from a to b into a number of segments ($\boldsymbol{N}$).
- The areas of individual segment can then be added to yield the integral for the entire interval.
- There are $\boldsymbol{N+1}$ equally spaced nodes

$$x_0, x_1, \dots\dots, x_N$$

- Let, $x_0 = a \; and \; x_N = b$

- Assume, $x_k = x_0 + kh, k = 0, 1, 2, \ldots., N$ are equally spaced nodes.

- Thus, $h = \frac{b-a}{N}$

- Therefore

$$\int_a^b f(x) \quad dx = \int_{x_0}^{x_1} f(x) \quad dx + \int_{x_1}^{x_2} f(x) \quad dx + \ldots + \int_{x_{N-1}}^{x_N} f(x) \quad dx$$

with

$$\int_{x_k}^{x_{k+1}} f(x) \quad dx \approx \int_{x_k}^{x_{k+1}} p_n(x) \quad dx$$

- Let, $p_n(x) = f_k + r\Delta f_k$

with $x = x_k + rh \quad (dx = hdr)$

- Thus, $\int_{x_k}^{x_{k+1}} f(x) \ dx \approx \int_{x_k}^{x_{k+1}} p_n(x) \ dx$

$$= \int_{x_k}^{x_k+h} \left(f_k + r\Delta f_k \right) \ dx$$

$$= h\int_0^1 \left(f_k + r\Delta f_k \right) \ dr$$

$$= h\left(rf_k + \frac{r^2}{2}\Delta f_k \right)\Bigg|_0^1 \qquad = h\left(f_k + \frac{1}{2}\Delta f_k \right)$$

$$= h\left[f_k + \frac{1}{2}\left(f_{k+1} - f_k \right) \right]$$

$$= \frac{h}{2}\left(f_k + f_{k+1} \right)$$

$$\int_a^b f(x)\ dx \approx \frac{h}{2}\left(f_0 + f_1\right) + \frac{h}{2}\left(f_1 + f_2\right) + \ldots + \frac{h}{2}\left(f_{N-1} + f_N\right)$$

$$= \frac{h}{2}\left(f_0 + 2f_1 + 2f_2 + \ldots + 2f_{N-1} + f_N\right)$$

$$\boxed{\int_a^b f(x)\ dx = \frac{h}{2}\left(f_0 + f_N + 2\sum_{i=1}^{N-1} f_i\right)}$$

Formula of Trapezoidal Rule

Example

Approximate the following integral using the Trapezoidal rule with h = 0.5 and h = 0.25.

$$\int_1^4 \frac{x}{\sqrt{x+4}} \, dx$$

Example - Solution

$$\int_1^4 \frac{x}{\sqrt{x+4}}\,dx$$

For $h=0.5$:

Step 1: Calculate N

$a = 1$; $b = 4$

$$N = \frac{b-a}{h} = \frac{4-1}{0.5} = 6$$

Step 2: Calculate $f(x_i)$

i	x_i	$f(x_i) = \frac{x_i}{\sqrt{x_i+4}}$	
0	1.0	0.4472	
1	1.5		0.6396
2	2.0		0.8165
3	2.5		0.9806
4	3.0		1.1339
5	3.5		1.2780
6	4.0	1.4142	
	Total	1.8614	4.8486

Example - Solution (cont'd)

$$\int_1^4 \frac{x}{\sqrt{x+4}} \, dx = \int_1^4 f(x) \, dx$$

$$= \frac{h}{2}\left[f_0 + f_6 + 2\left(f_1 + f_2 + f_3 + f_4 + f_5 \right) \right]$$

$$= \frac{0.5}{2}\left[1.8614 + 2(4.8486)\right]$$

$$= 2.8896$$

Example – Solution (cont'd)

$$\int_1^4 \frac{x}{\sqrt{x+4}} \quad dx$$

For $h=0.25$:

Step 1: Calculate N

$a = 1$; $b = 4$

$$N = \frac{b-a}{h} = \frac{4-1}{0.25} = 12$$

Step 2: Calculate $f(x_i)$

i	x_i	$f(x_i) = \frac{x_i}{\sqrt{x_i + 4}}$	
0	1.00	0.4472	
1	1.25		0.5455
2	1.50		0.6396
3	1.75		0.7298
4	2.00		0.8165
5	2.25		0.9000
6	2.50		0.9806
7	2.75		1.0585
8	3.00		1.1339
9	3.25		1.2070
10	3.50		1.2780
11	3.75		1.3470
12	4.00	1.4142	
	Total	1.8614	10.6364

Example – Solution (cont'd)

$$\int_1^4 \frac{x}{\sqrt{x+4}} \, dx = \int_1^4 f(x) \, dx$$

$$= \frac{h}{2}\left[f_0 + f_{12} + 2\sum_{i=1}^{11} f_i \right]$$

$$= \frac{0.25}{2}\left[1.8614 + 2(10.6364)\right]$$

$$= 2.8918$$

(Note: The exact value of the integral is 2.8925)

- For h=0.5, N=6, the error is 0.0029
- For h=0.25, N=12, the error is 0.0007

- The error decreases as the number of segments (N) increases.
- When h is reduced by a factor of ½ the successive errors are diminished by approximately ¼.

Exercise 1

Approximate the following integrals using the **Trapezoidal rule** with N=10.

(a) $\int_0^2 e^x \, dx$ (b) $\int_1^2 \sqrt{x^3 - 1} \, dx$

Simpson’s Rule

- The trapezoidal rule usually requires a large number of function evaluations to achieve an accurate answer.

- Another way to obtain a more accurate estimate of an integral is to use higher-order polynomials to connect the points.

- Let, $p_2(x) = f_k + r\Delta f_k + \frac{1}{2}r(r-1)\Delta^2 f_k$

$$\int_{x_k}^{x_{k+2}} f(x)\ dx = \int_{x_k}^{x_k+2h} \left(f_k + r\Delta f_k + \frac{1}{2}r(r-1)\Delta^2 f_k \right) dx$$

$$= h\int_0^2 \left(f_k + r\Delta f_k + \frac{1}{2}r(r-1)\Delta^2 f_k \right) dr$$

$$= h\left(rf_k + \frac{r^2}{2}\Delta f_k + \frac{1}{2}\left(\frac{r^3}{3} - \frac{r^2}{2}\right)\Delta^2 f_k \right)\Bigg|_0^2$$

$$= h\left(2f_k + 2\Delta f_k + \frac{1}{3}\Delta^2 f_k\right)$$

$$= h\left(2f_k + 2\left(f_{k+1} - f_k\right) + \frac{1}{3}\left(f_{k+2} - 2f_{k+1} + f_k\right)\right)$$

$$= \frac{h}{3}\left(f_k + 4f_{k+1} + f_{k+2}\right)$$

- Subdivide the interval $[a,b]$ into N subintervals (N is even).

$$\int_a^b f(x)\ dx = \int_{x_0}^{x_2} f(x)\ dx + \int_{x_2}^{x_4} f(x)\ dx + \ldots + \int_{x_{N-2}}^{x_N} f(x)\ dx$$

$$= \frac{h}{3}\left(f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \ldots + 4f_{N-1} + f_N \right)$$

- This equation is known as **Simpson's 1/3 rule.**

$$\int_a^b f(x) \quad dx = \frac{h}{3}\left[\left(f_0 + f_N \right) + 4\sum_{i=1}^{N/2} f_{2i-1} + 2\sum_{i=1}^{N/2-1} f_{2i} \right]$$

where N is even.

Simpson's 3/8 Rule

- Let,

$$p_3(x) = f_k + r\Delta f_k + \frac{1}{2} r(r-1)\Delta^2 f_k + \frac{1}{6} r(r-1)(r-2)\Delta^3 f_k$$

$$\int_{x_k}^{x_{k+3}} f(x) \quad dx = \int_{x_k}^{x_{k+3}} p_3(x) \quad dx$$

$$\int_a^b f(x)\;\; dx = \frac{3h}{8}\left[\left(f_0 + f_N\right) + 3\sum_{i=1}^{N/3}\left(f_{3i-2} + f_{3i-1}\right) + 2\sum_{i=1}^{N/3-1} f_{3i} \right]$$

where N = 3, 6, 9, 12, ...

- This equation is called **Simpson's 3/8 rule** because *h* is multiplied by 3/8.

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Example

Approximate the following integrals using the Simpson's 1/3 rule with h=0.5 and h=0.25.

$$\int_1^4 \frac{x}{\sqrt{x+4}} \, dx$$

Example - Solution

$$\int_1^4 \frac{x}{\sqrt{x+4}}\ dx$$

For h=0.5:

Step 1: Calculate N.

$a = 1$; $b = 4$

$$N = \frac{b-a}{h} = \frac{4-1}{0.5} = 6$$

(N is even)

Example – Solution (cont'd)

Step 2: Calculate $f(x_i)$

i	x_i	$f_i = f(x_i) = \dfrac{x_i}{\sqrt{x_i + 4}}$		
0	1.0	0.4472		
1	1.5		0.6396	
2	2.0			0.8165
3	2.5		0.9806	
4	3.0			1.1339
5	3.5		1.2780	
6	4.0	1.4142		
	Total	1.8614	2.8982	1.9504

Example – Solution (cont'd)

$$\int_1^4 \frac{x}{\sqrt{x+4}}\,dx = \frac{h}{3}\left[(f_0 + f_6) + 4\sum_{i=1}^{3} f_{2i-1} + 2\sum_{i=1}^{2} f_{2i} \right]$$

$$= \frac{0.5}{3}\left[1.8614 + 4(2.8982) + 2(1.9504)\right]$$

$$= 2.8925$$

Example – Solution (cont'd)

For $h=0.25$:

Step 1: Calculate N.

$a = 1$; $b = 4$

$$N = \frac{b-a}{h} = \frac{4-1}{0.25} = 12$$

(*N* is even)

Step 2:

Calculate $f(x_i)$

i	x_i	$f_i = f(x_i) = \frac{x_i}{\sqrt{x_i + 4}}$		
0	1.00	0.4472		
1	1.25		0.5455	
2	1.50			0.6396
3	1.75		0.7298	
4	2.00			0.8165
5	2.25		0.9000	
6	2.50			0.9806
7	2.75		1.0585	
8	3.00			1.1339
9	3.25		1.2070	
10	3.50			1.2780
11	3.75		1.3470	
12	4.00	1.4142		
	Total	1.8614	5.7878	4.8486

Example – Solution (cont'd)

$$\int_1^4 \frac{x}{\sqrt{x+4}}\,dx = \frac{h}{3}\left[\left(f_0 + f_{12}\right) + 4\sum_{i=1}^{6} f_{2i-1} + 2\sum_{i=1}^{5} f_{2i}\right]$$

$$= \frac{0.25}{3}\left[1.8614 + 4(5.7878) + 2(4.8486)\right]$$

$$= 2.8925$$

Example

Approximate the following integrals using the Simpson's 3/8 rule with h=0.25.

$$\int_1^4 \frac{x}{\sqrt{x+4}} \, dx$$

Example – Solution

For $h=0.25$:

Step 1: Calculate N.

$a = 1 \; ; \; b = 4$

$$N = \frac{b-a}{h} = \frac{4-1}{0.25} = 12$$

Step 2:

Calculate $f(x_i)$

i	x_i	$f_i = f(x_i) = \dfrac{x_i}{\sqrt{x_i + 4}}$		
0	1.00	0.4472		
1	1.25		0.5455	
2	1.50		0.6396	
3	1.75			0.7298
4	2.00		0.8165	
5	2.25		0.9000	
6	2.50			0.9806
7	2.75		1.0586	
8	3.00		1.1339	
9	3.25			1.2070
10	3.50		1.2780	
11	3.75		1.3470	
12	4.00	1.4142		
	Total	1.8614	7.7191	2.9174

Example – Solution (cont'd)

$$\int_1^4 \frac{x}{\sqrt{x+4}}\,dx = \frac{3h}{8}\left[(f_0 + f_{12}) + 3\sum_{i=1}^{4}(f_{3i-2} + f_{3i-1}) + 2\sum_{i=1}^{3} f_{3i}\right]$$

$$= \frac{3(0.25)}{8}\left[1.8614 + 3(7.7191) + 2(2.9174)\right]$$

$$= 2.8925$$

- Simpson's 1/3 rule is usually the method of preference because it attains third-order accuracy with three points rather than the four points required for the 3/8 version.

Exercise 2

Approximate the following integral

$$\int_0^3 \frac{1}{\sqrt{x^3+1}}\,dx$$

using

a) **The Simpson's 1/3 rule**

b) **The Simpson's 3/8 rule**

with N=12.

Romberg Integration

Romberg integration uses the Trapezoidal rule to give preliminary approximations and then applies the Richardson extrapolation process to improve the approximations.

- The first step in the Romberg process obtains the Trapezoidal rule approximations.

- Start with 1 subinterval, $h_1 = b - a$

$$R_{1,1} = \frac{h_1}{2}\left(f_0 + f_1\right)$$

- For N_i subintervals, $N_i=2^{i-1}$ (e.g., $N_2=2$, $N_3=4$, $N_4=8$)

$$h_i = \frac{1}{2} h_{i-1} \qquad \text{or} \qquad h_i = \frac{b-a}{2^{i-1}}$$

$$\boxed{R_{i,1} = \frac{1}{2}\left[R_{i-1,1} + h_{i-1} \sum_{k=1}^{2^{i-2}} f_{2k-1} \right]} \qquad i = 2, 3, \ldots$$

- Example: for i=2, $N_2=2^{2-1}=2$

$$h_2 = \frac{1}{2} h_1$$

$$R_{2,1} = h_2 \left[\frac{1}{2} \left(f_0 + f_2 \right) + f_1 \right]$$

$$R_{2,1} = h_2\left[\frac{1}{2}\left(f_0 + f_2\right) + f_1\right] \quad = \frac{h_1}{2}\left[\frac{1}{2}\left(f_0 + f_2\right) + f_1\right]$$

$$= \frac{1}{2}\left[\frac{h_1}{2}\left(f_0 + f_2\right) + h_1 f_1\right] = \frac{1}{2}\left[R_{1,1} + h_1 f_1\right]$$

$$= \frac{1}{2}\left[R_{1,1} + h_1 \sum_{k=1}^{1} f_{2k-1}\right]$$

- Example: for i=3, $N_3=2^{3-1}=4$

$$h_3 = \frac{1}{2} h_2$$

$$R_{3,1} = h_3 \left[\frac{1}{2}\left(f_0 + f_4 \right) + f_1 + f_2 + f_3 \right]$$

$$R_{3,1} = h_3\left[\frac{1}{2}\left(f_0 + f_4\right) + f_1 + f_2 + f_3\right]$$

$$= \frac{h_2}{2}\left[\frac{1}{2}\left(f_0 + f_4\right) + f_1 + f_2 + f_3\right]$$

$$= \frac{1}{2}\left[\frac{h_2}{2}\left(f_0 + f_4\right) + h_2 f_2 + h_2\left(f_1 + f_3\right)\right]$$

$$= \frac{1}{2}\left[R_{2,1} + h_2\left(f_1 + f_3\right)\right] \qquad = \frac{1}{2}\left[R_{2,1} + h_2\sum_{k=1}^{2} f_{2k-1}\right]$$

$$R_{i,1} = \frac{1}{2}\left[R_{i-1,1} + h_{i-1}\sum_{k=1}^{2^{i-2}} f_{2k-1}\right]$$

- For i=2, 3, …

$$h_{i-1} = \frac{1}{2}h_{i-2}$$

- Richardson's improvement,

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

for $i = 2, 3, \ldots, N$ and $j = 2, 3 \ldots, i$.

$$R_{2,2} = \frac{4R_{2,1} - R_{1,1}}{3}$$

$$R_{3,2} = \frac{4R_{3,1} - R_{2,1}}{3}$$

$$R_{3,3} = \frac{16R_{3,2} - R_{2,2}}{15}$$

$$R_{4,4} = \frac{64R_{4,3} - R_{3,3}}{63}$$

Romberg Table

i	$h_i = \dfrac{b-a}{2^{i-1}}$	$R_{i,1}$	$R_{i,2}$	$R_{i,3}$	$\dots$	$R_{i,N}$
1	h_1	$R_{1,1}$				
2	h_2	$R_{2,1}$	$R_{2,2}$			
3	h_3	$R_{3,1}$	$R_{3,2}$	$R_{3,3}$		
$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	
N	h_N	$R_{N,1}$	$R_{N,2}$	$R_{N,3}$	$\dots$	$R_{N,N}$

Compute the Romberg table until $|R_{i,j} - R_{i,j-1}| < \varepsilon$

Example

Use Romberg integration to approximate

$$\int_1^4 \frac{x}{\sqrt{x+4}} \, dx$$

Compute the Romberg table until $|R_{i,j} - R_{i,j-1}| < 0.0005$

Example – Solution

$$h_1 = b - a = 4 - 1 = 3$$

1) $$R_{1,1} = \frac{h_1}{2}\left(f_0 + f_1\right)$$

$$= \frac{3}{2}\left(0.4472 + 1.4142\right)$$

$$= 2.7921.$$

Example – Solution (cont'd)

2) $$R_{2,1}=\frac{1}{2}\left[R_{1,1}+h_1\sum_{k=1}^{1} f_{2k-1}\right]$$

$$=\frac{1}{2}\left[R_{1,1}+h_1(f_1)\right]=\frac{1}{2}\left[R_{1,1}+h_1(f(2.5))\right]$$

$$=\frac{1}{2}\left[2.7921+3(0.9806)\right]=2.8670$$

3) $$R_{2,2}=\frac{4R_{2,1}-R_{1,1}}{3}=\frac{4(2.8670)-2.7921}{3}=2.8920$$

4) $$\left|R_{2,2}-R_{2,1}\right|=\left|2.8920-2.8670\right|=0.025>0.0005$$

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Example – Solution (cont'd)

5) $$R_{3,1} = \frac{1}{2}\left[R_{2,1} + h_2 \sum_{k=1}^{2} f_{2k-1}\right] = \frac{1}{2}\left[R_{2,1} + h_2 (f_1 + f_3)\right]$$

$$= \frac{1}{2}\left[R_{2,1} + h_2 (f(1.75) + f(3.25))\right]$$

$$= \frac{1}{2}\left[2.8670 + 1.5(0.7298 + 1.2070)\right] = 2.8861$$

Example – Solution (cont'd)

6) $$R_{3,2}=\frac{4R_{3,1}-R_{2,1}}{3}=\frac{4(2.8861)-2.8670}{3}=2.8925$$

7) $$\left|R_{3,2}-R_{3,1}\right|=\left|2.8925-2.8861\right|=0.0064>0.0005$$

8) $$R_{3,3}=\frac{16R_{3,2}-R_{2,2}}{15}=\frac{16(2.8925)-2.8920}{15}=2.8925$$

9) $$\left|R_{3,3}-R_{3,2}\right|=\left|2.8925-2.8925\right|=0.0000<0.0005$$ (calculation can be stopped.)

Example – Solution (cont'd)

- The Romberg table:

i	$h_i = \frac{b-a}{2^{i-1}}$	$R_{i,1}$	$R_{i,2}$	$R_{i,3}$
1	3	2.7921		
2	1.5	2.8670	2.8920	
3	0.75	2.8861	2.8925	2.8925

- The solution is,

$$\int_1^4 \frac{x}{\sqrt{x+4}}\, dx = R_{3,3} = 2.8925$$

Exercise 3

Use **Romberg** integration to approximate:

(a) $\int_0^2 (4 - x^2)^{1/2}\, dx$

(b) $\int_0^{\pi} \sin x \quad dx$

Compute the Romberg table until $|R_{i,j} - R_{i,j\text{-}1}| < 0.005$