Differentiation and Integration

Numerical differentiation

Three-Point Endpoint Formula

- $$f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)] + \frac{h^2}{3} f^{(3)}(\xi_0), \qquad (4.4)$$

where ξ_0 lies between x_0 and $x_0 + 2h$.

Three-Point Midpoint Formula

- $$f'(x_0) = \frac{1}{2h}[f(x_0 + h) - f(x_0 - h)] - \frac{h^2}{6} f^{(3)}(\xi_1), \qquad (4.5)$$

where ξ_1 lies between $x_0 - h$ and $x_0 + h$.

Five-Point Endpoint Formula

- $$f'(x_0) = \frac{1}{12h}[-25f(x_0) + 48f(x_0+h) - 36f(x_0+2h) + 16f(x_0+3h) - 3f(x_0+4h)] + \frac{h^4}{5}f^{(5)}(\xi), \tag{4.7}$$

  where ξ lies between x_0 and $x_0 + 4h$.

Five-Point Midpoint Formula

- $$f'(x_0) = \frac{1}{12h}[f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)] + \frac{h^4}{30}f^{(5)}(\xi), \tag{4.6}$$

  where ξ lies between $x_0 - 2h$ and $x_0 + 2h$.

Second Derivative Midpoint Formula

- $$f''(x_0) = \frac{1}{h^2}[f(x_0 - h) - 2f(x_0) + f(x_0 + h)] - \frac{h^2}{12}f^{(4)}(\xi), \qquad (4.9)$$

  for some ξ, where $x_0 - h < \xi < x_0 + h$.

Example 3 In Example 2 we used the data shown in Table 4.3 to approximate the first derivative of $f(x) = xe^x$ at $x = 2.0$. Use the second derivative formula (4.9) to approximate $f''(2.0)$.

Table 4.3

x	$f(x)$
1.8	10.889365
1.9	12.703199
2.0	14.778112
2.1	17.148957
2.2	19.855030

$$\frac{1}{0.01}[f(1.9) - 2f(2.0) + f(2.1)] = 100[12.703199 - 2(14.778112) + 17.148957]$$
$$= 29.593200,$$

$$\frac{1}{0.04}[f(1.8) - 2f(2.0) + f(2.2)] = 25[10.889365 - 2(14.778112) + 19.855030]$$
$$= 29.704275.$$

Because $f''(x) = (x + 2)e^x$, the exact value is $f''(2.0) = 29.556224$. Hence the actual errors are -3.70×10^{-2} and -1.48×10^{-1}, respectively. ■

Class Activity Exercise 4.1

1. Use the forward-difference formulas and backward-difference formulas to determine each missing entry in the following tables.

a.

x	$f(x)$	$f'(x)$
0.5	0.4794	
0.6	0.5646	
0.7	0.6442	

b.

x	$f(x)$	$f'(x)$
0.0	0.00000	
0.2	0.74140	
0.4	1.3718	

5. Use the most accurate three-point formula to determine each missing entry in the following tables.

a.

x	$f(x)$	$f'(x)$
1.1	9.025013	
1.2	11.02318	
1.3	13.46374	
1.4	16.44465	

b.

x	$f(x)$	$f'(x)$
8.1	16.94410	
8.3	17.56492	
8.5	18.19056	
8.7	18.82091	

Class Activity

6. Use the most accurate three-point formula to determine each missing entry in the following tables.

a.

x	$f(x)$	$f'(x)$
-0.3	-0.27652	
-0.2	-0.25074	
-0.1	-0.16134	
0	0	

b.

x	$f(x)$	$f'(x)$
7.4	-68.3193	
7.6	-71.6982	
7.8	-75.1576	
8.0	-78.6974	

c.

x	$f(x)$	$f'(x)$
1.1	1.52918	
1.2	1.64024	
1.3	1.70470	
1.4	1.71277	

d.

x	$f(x)$	$f'(x)$
-2.7	0.054797	
-2.5	0.11342	
-2.3	0.65536	
-2.1	0.98472	

7. The data in Exercise 5 were taken from the following functions. Compute the actual errors in Exercise 5, and find error bounds using the error formulas.

a. $f(x) = e^{2x}$

b. $f(x) = x \ln x$

c. $f(x) = x \cos x - x^2 \sin x$

d. $f(x) = 2(\ln x)^2 + 3 \sin x$

8. The data in Exercise 6 were taken from the following functions. Compute the actual errors in Exercise 6, and find error bounds using the error formulas.

a. $f(x) = e^{2x} - \cos 2x$

b. $f(x) = \ln(x + 2) - (x + 1)^2$

c. $f(x) = x \sin x + x^2 \cos x$

d. $f(x) = (\cos 3x)^2 - e^{2x}$

Class Activity-HW

18. Consider the following table of data:

x	0.2	0.4	0.6	0.8	1.0
$f(x)$	0.9798652	0.9177710	0.808038	0.6386093	0.3843735

a. Use all the appropriate formulas given in this section to approximate $f'(0.4)$ and $f''(0.4)$.

b. Use all the appropriate formulas given in this section to approximate $f'(0.6)$ and $f''(0.6)$.

20. Let $f(x) = 3xe^x - \cos x$. Use the following data and Eq. (4.9) to approximate $f''(1.3)$ with $h = 0.1$ and with $h = 0.01$.

x	1.20	1.29	1.30	1.31	1.40
$f(x)$	11.59006	13.78176	14.04276	14.30741	16.86187

Compare your results to $f''(1.3)$.

Three approximations to the derivative $f'(a)$ are

1. the one sided (forward) difference $$\frac{f(a+h)-f(a)}{h}$$

2. the one sided (backward) difference $$\frac{f(a)-f(a-h)}{h}$$

3. the central difference $$\frac{f(a+h)-f(a-h)}{2h}$$

   (Mid Point)

A central difference approximation to the second derivative $f''(a)$ is

$$f''(a) \approx \frac{f(a+h)-2f(a)+f(a-h)}{h^2}$$

Class Activity

Example The distance x of a runner from a fixed point is measured (in metres) at intervals of half a second. The data obtained is

t	0.0	0.5	1.0	1.5	2.0
x	0.00	3.65	6.80	9.90	12.15

Use central differences to approximate the runner's velocity at times $t = 0.5$s and $t = 1.25$s.

Solution

Our aim here is to approximate $x'(t)$. The choice of h is dictated by the available data. Using data with $t = 0.5$s at its centre we obtain

$$x'(0.5) \approx \frac{x(1.0) - x(0.0)}{2 \times 0.5} = 6.80\text{m/s}.$$

Data centred at $t = 1.25$s gives us the approximation

$$x'(1.25) \approx \frac{x(1.5) - x(1.0)}{2 \times 0.25} = 6.20\text{m/s}.$$

Class Activity

Example The distance x of a runner from a fixed point is measured (in metres) at intervals of half a second. The data obtained is

t	0.0	0.5	1.0	1.5	2.0
x	0.00	3.65	6.80	9.90	12.15

Use a central difference to approximate the runner's acceleration at time $t =$ 1.5s.

Solution

Our aim here is to approximate $x''(t)$.
Using data with $t = 1.5$s at its centre we obtain

$$x''(1.5) \approx \frac{x(2.0) - 2x(1.5) + x(1.0)}{0.5^2} = -3.40\text{m/s}^2,$$

Class Activity

The velocity v (in m/s) of a rocket measured at half second intervals is

t	0.0	0.5	1.0	1.5	2.0
v	0.000	11.860	26.335	41.075	59.051

Use central differences to approximate the acceleration of the rocket at times $t = 1.0$s and $t = 1.75$s.

Using data with $t = 1.0$s at its centre we obtain

$$v'(1.0) \approx \frac{v(1.5) - v(0.5)}{1.0} = 29.215\text{m/s}^2.$$

Data centred at $t = 1.75$s gives us the approximation

$$v'(1.75) \approx \frac{v(2.0) - v(1.5)}{0.5} = 35.952\text{m/s}^2.$$

CLASS_ACTIVITY

The distance x, measured in metres, of a downhill skier from a fixed point is measured at intervals of 0.25 s. The data gathered is

t	0	0.25	0.5	0.75	1	1.25	1.5
x	0	4.3	10.2	17.2	26.2	33.1	39.1

Use a central difference to approximate the skier's velocity and acceleration at the times t =0.25s, 0.75s and 1.25s. Give your answers to 1 decimal place.

CLASS_ACTIVITY

The distance $D = D(t)$ traveled by an object is given in the table following.

t	$D(t)$
8.0	17.453
9.0	21.460
10.0	25.752
11.0	30.301
12.0	35.084

(a) Find the velocity $V(10)$ by numerical differentiation.

(b) Compare your answer with $D(t) = -70 + 7t + 70e^{-t/10}$.

c) Find velocity and acceleration at t=10 using midpoint formula

The Trapezoidal Rule (Composite Form)

The Newton-Cotes formula is based on approximating y = f (x) between (x_0, y_0) and (x_1, y_1)by a straight line, thus forming a trapezium, is called trapezoidal rule. In order to evaluate the definite integral

$$I = \int_a^b f(x)dx$$

we divide the interval [a, b] into n sub-intervals, each of size $h = (b - a)/n$ and denote the sub-intervals by $[x_0, x_1]$, $[x_1, x_2]$, …, $[x_{n-1}, x_n]$, such that $x_0 = a$ and $x_n = b$ and $x_k = x_0 + k_h$, $k = 1, 2, \ldots, n - 1$.

Thus, we can write the above definite integral as a sum. Therefore,

$$I = \int_{x_0}^{x_n} f(x)dx = \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)dx$$

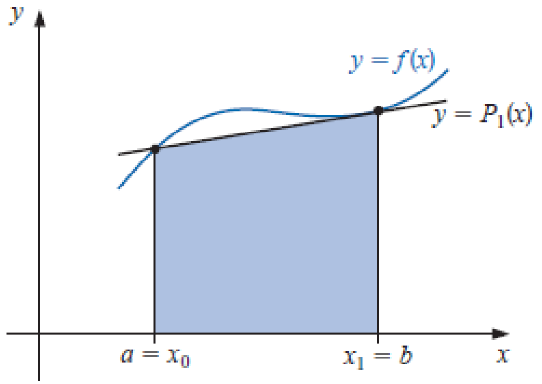
$$\int_{x_0}^{x_n} f(x)dx = \frac{h}{2}(y_0 + 2y_1 + 2y_2 + \cdots + 2y_{n-1} + y_n) + E_n$$

Derivation:

The Trapezoidal Rule

To derive the Trapezoidal rule for approximating $\int_a^b f(x)\,dx$, 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

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_1} \left[\frac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)} f(x_1) \right] dx$$

$$\int_a^b f(x)\,dx = \left[\frac{(x - x_1)^2}{2(x_0 - x_1)} f(x_0) + \frac{(x - x_0)^2}{2(x_1 - x_0)} f(x_1) \right]_{x_0}^{x_1} = \frac{(x_1 - x_0)}{2}[f(x_0) + f(x_1)] = \frac{h}{2}[f(x_0) + f(x_1)]$$

Similarly $\int_{x1}^{x2} f(x)dx = \frac{h}{2}[f(x1) + f(x2)$, *and* $\int_{x(n-1)}^{xn} f(x)dx = \frac{h}{2}[f(x_{n-1}) + f(xn)]$,

$$\int_{x_0}^{x_n} f(x)dx = \frac{h}{2}(y_0 + 2y_1 + 2y_2 + \cdots + 2y_{n-1} + y_n) + E_n$$

Is called trapezoidal rule

Simpson's Rules (Composite Forms)

the definite integral I can be written as

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

$$I = \frac{h}{3}[(y_0 + 4y_1 + y_2) + (y_2 + 4y_3 + y_4) + \cdots \quad + (y_{2N-2} + 4y_{2N-1} + y_{2N})]$$

$$\int_{x_0}^{x_{2N}} f(x)dx = \frac{h}{3}[y_0 + 4(y_1 + y_3 + \cdots + y_{2N-1}) + 2(y_2 + y_4 + \cdots + y_{2N-2}) + y_{2N}] + \text{Error term}$$

This formula is called composite Simpson's 1/3 rule.

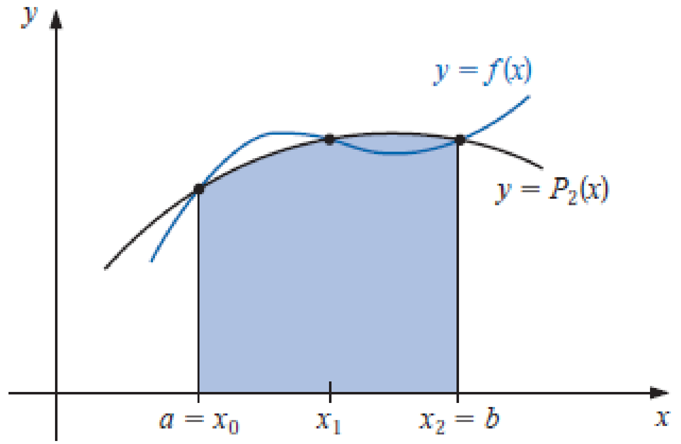
Derivation-1:

Simpson's Rule

Simpson's rule results from integrating over $[a, b]$ the second Lagrange polynomial with equally-spaced nodes $x_0 = a$, $x_2 = b$, and $x_1 = a + h$, where $h = (b - a)/2$. (See Figure 4.4.)

Therefore

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_2} \left[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \right] dx$$



$$\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)]$$

similarly $\int_{x2}^{x4} f(x)dx = \frac{h}{3}[f(x2) + 4f(x3) + f(x4)]$ and

$$\int_{x_0}^{x_{2N}} f(x)dx = \frac{h}{3}[y_0 + 4(y_1 + y_3 + \cdots + y_{2N-1}) + 2(y_2 + y_4 + \cdots + y_{2N-2}) + y_{2N}] + \text{Error term}$$

Is called Simpson's rule

Derivation-2:

Similarly in deriving composite Simpson's 3/8 rule, we divide the interval of integration into n sub-intervals, where n is divisible by 3, and applying the integration formula

$$\int_{x_0}^{x_n} f(x)dx = \int_{x_0}^{x_3} f(x)dx + \int_{x_3}^{x_6} f(x)dx + \cdots + \int_{x_{n-3}}^{x_n} f(x)dx$$

$$\int_{x_0}^{x_3} f(x)dx = \frac{3}{8}h(y_0 + 3y_1 + 3y_2 + y_3)$$

We obtain the composite form of Simpson's 3/8 rule as

$$\int_a^b f(x)dx = \frac{3}{8}h[y(a) + 3y_1 + 3y_2 + 2y_3 + 3y_4 + 3y_5 + 2y_6 + \cdots$$

$$+ 2y_{n-3} + 3y_{n-2} + 3y_{n-1} + y(b)]$$

Quadrature formula in term of sigma notation

TRAPEZOIDAL RULE

$$\int_{x_0}^{x_n} f(x)dx = \frac{h}{2}(y_0 + 2y_1 + 2y_2 + \cdots + 2y_{n-1} + y_n) + E_n$$

$$T(f,h) = \frac{h}{2}(f(a) + f(b)) + h\sum_{k=1} f(x_k).$$

SIMPSON'S 1/3 RULE

$$\int_{x_0}^{x_{2N}} f(x)dx = \frac{h}{3}[y_0 + 4(y_1 + y_3 + \cdots + y_{2N-1}) + 2(y_2 + y_4 + \cdots + y_{2N-2}) + y_{2N}] + \text{Error term}$$

$$S(f,h) = \frac{h}{3}(f(a) + f(b)) + \frac{2h}{3}\sum_{k=1}^{M-1} f(x_{2k}) + \frac{4h}{3}\sum_{k=1}^{M} f(x_{2k-1}).$$

Simpson's 3/8 rule is

$$\int_a^b f(x)dx = \frac{3}{8}h[y(a) + 3y_1 + 3y_2 + 2y_3 + 3y_4 + 3y_5 + 2y_6 + \cdots + 2y_{n-3} + 3y_{n-2} + 3y_{n-1} + y(b)]$$

Closed-Newton-Cotes (Quadrature formulas)

Theorem 4.2 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

N=1

$$\int_{x_0}^{x_1} f(x)\,dx \approx \frac{h}{2}(f_0 + f_1)$$ (the trapezoidal rule),

N=2

$$\int_{x_0}^{x_2} f(x)\,dx \approx \frac{h}{3}(f_0 + 4f_1 + f_2)$$ (Simpson's rule),

N=3

$$\int_{x_0}^{x_3} f(x)\,dx \approx \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3)$$ (Simpson's $\frac{3}{8}$ rule),

N=4

$$\int_{x_0}^{x_4} f(x)\,dx \approx \frac{2h}{45}(7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4)$$

(Boole's rule).

Open-Newton-Cotes formulas

Theorem 4.3 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

$n = 0$: Midpoint rule

$$\int_{x_{-1}}^{x_1} f(x)\,dx = 2hf(x_0).$$

$n = 1$:

$$\int_{x_{-1}}^{x_2} f(x)\,dx = \frac{3h}{2}[f(x_0) + f(x_1)]$$

$n = 2$:

$$\int_{x_{-1}}^{x_3} f(x)\,dx = \frac{4h}{3}[2f(x_0) - f(x_1) + 2f(x_2)].$$

$n = 3$:

$$\int_{x_{-1}}^{x_4} f(x)\,dx = \frac{5h}{24}[11f(x_0) + f(x_1) + f(x_2) + 11f(x_3)].$$

Class Activity

Example 2 Compare the results of the closed and open Newton-Cotes formulas listed as (4.25)–(4.28) and (4.29)–(4.32) when approximating

$$\int_0^{\pi/4} \sin x \, dx = 1 - \sqrt{2}/2 \approx 0.29289322.$$

Calculate true error by both methods

Example 2 Compare the results of the closed and open Newton-Cotes formulas listed as (4.25)–(4.28) and (4.29)–(4.32) when approximating

$$\int_0^{\pi/4} \sin x \, dx = 1 - \sqrt{2}/2 \approx 0.29289322.$$

Solution For the closed formulas we have

$$n = 1: \quad \frac{(\pi/4)}{2}\left[\sin 0 + \sin \frac{\pi}{4}\right] \approx 0.27768018$$

$$n = 2: \quad \frac{(\pi/8)}{3}\left[\sin 0 + 4\sin \frac{\pi}{8} + \sin \frac{\pi}{4}\right] \approx 0.29293264$$

$$n = 3: \quad \frac{3(\pi/12)}{8}\left[\sin 0 + 3\sin \frac{\pi}{12} + 3\sin \frac{\pi}{6} + \sin \frac{\pi}{4}\right] \approx 0.29291070$$

$$n = 4: \quad \frac{2(\pi/16)}{45}\left[7\sin 0 + 32\sin \frac{\pi}{16} + 12\sin \frac{\pi}{8} + 32\sin \frac{3\pi}{16} + 7\sin \frac{\pi}{4}\right] \approx 0.29289318$$

and for the open formulas we have

$$n = 0: \quad 2(\pi/8)\left[\sin \frac{\pi}{8}\right] \approx 0.30055887$$

$$n = 1: \quad \frac{3(\pi/12)}{2}\left[\sin \frac{\pi}{12} + \sin \frac{\pi}{6}\right] \approx 0.29798754$$

$$n = 2: \quad \frac{4(\pi/16)}{3}\left[2\sin \frac{\pi}{16} - \sin \frac{\pi}{8} + 2\sin \frac{3\pi}{16}\right] \approx 0.29285866$$

$$n = 3: \quad \frac{5(\pi/20)}{24}\left[11\sin \frac{\pi}{20} + \sin \frac{\pi}{10} + \sin \frac{3\pi}{20} + 11\sin \frac{\pi}{5}\right] \approx 0.29286923$$

Class Activity

Example :

Evaluate the integral $I = \int_0^1 \frac{dx}{1+x^2}$

Example: Compute the integral $I = \sqrt{\frac{2}{\pi}} \int_0^1 e^{-x^2/2} dx$ using Simpson's 1/3 rule,

Taking h = 0.125.

Exercises (HW)

4.3

1. Approximate the following integrals using the Trapezoidal rule.

a. $\int_{0.5}^{1} x^4\,dx$

b. $\int_{0}^{0.5} \frac{2}{x-4}\,dx$

c. $\int_{1}^{1.5} x^2 \ln x\,dx$

d. $\int_{0}^{1} x^2 e^{-x}\,dx$

e. $\int_{1}^{1.6} \frac{2x}{x^2-4}\,dx$

f. $\int_{0}^{0.35} \frac{2}{x^2-4}\,dx$

g. $\int_{0}^{\pi/4} x \sin x\,dx$

h. $\int_{0}^{\pi/4} e^{3x} \sin 2x\,dx$

2. Approximate the following integrals using the Trapezoidal rule.

a. $\int_{-0.25}^{0.25} (\cos x)^2\,dx$

b. $\int_{-0.5}^{0} x \ln(x+1)\,dx$

c. $\int_{0.75}^{1.3} \left((\sin x)^2 - 2x \sin x + 1\right)\,dx$

d. $\int_{e}^{e+1} \frac{1}{x \ln x}\,dx$

Exercises (HW)

4.4

1. Use the Composite Trapezoidal rule with the indicated values of n to approximate the following integrals.

   a. $\int_1^2 x \ln x \, dx, \quad n = 4$

   b. $\int_{-2}^2 x^3 e^x \, dx, \quad n = 4$

   c. $\int_0^2 \frac{2}{x^2+4} \, dx, \quad n = 6$

   d. $\int_0^\pi x^2 \cos x \, dx, \quad n = 6$

   e. $\int_0^2 e^{2x} \sin 3x \, dx, \quad n = 8$

   f. $\int_1^3 \frac{x}{x^2+4} \, dx, \quad n = 8$

   g. $\int_3^5 \frac{1}{\sqrt{x^2-4}} \, dx, \quad n = 8$

   h. $\int_0^{3\pi/8} \tan x \, dx, \quad n = 8$

2. Use the Composite Trapezoidal rule with the indicated values of n to approximate the following integrals.

   a. $\int_{-0.5}^{0.5} \cos^2 x \, dx, \quad n = 4$

   b. $\int_{-0.5}^{0.5} x \ln(x+1) \, dx, \quad n = 6$

   c. $\int_{.75}^{1.75} (\sin^2 x - 2x \sin x + 1) \, dx, \quad n = 8$

   d. $\int_e^{e+2} \frac{1}{x \ln x} \, dx, \quad n = 8$

3. Use the Composite Simpson's rule to approximate the integrals in Exercise 1.

2. *Length of a curve.* The arc length of the curve $y = f(x)$ over the interval $a \leq x \leq b$ is

$$\text{length} = \int_a^b \sqrt{1 + (f'(x)^2)}\, dx.$$

(i) Approximate the arc length of each function using the composite trapezoidal rule with $M = 10$.

(ii) Approximate the arc length of each function using the composite Simpson rule with $M = 5$.

(a) $f(x) = x^3$ for $0 \leq x \leq 1$

(b) $f(x) = \sin(x)$ for $0 \leq x \leq \pi/4$

(c) $f(x) = e^{-x}$ for $0 \leq x \leq 1$

3. *Surface area.* The solid of revolution obtained by rotating the region under the $y = f(x)$, where $a \leq x \leq b$, about the x-axis has surface area given by

$$\text{area} = 2\pi \int_a^b f(x)\sqrt{1 + (f'(x))^2}\, dx.$$