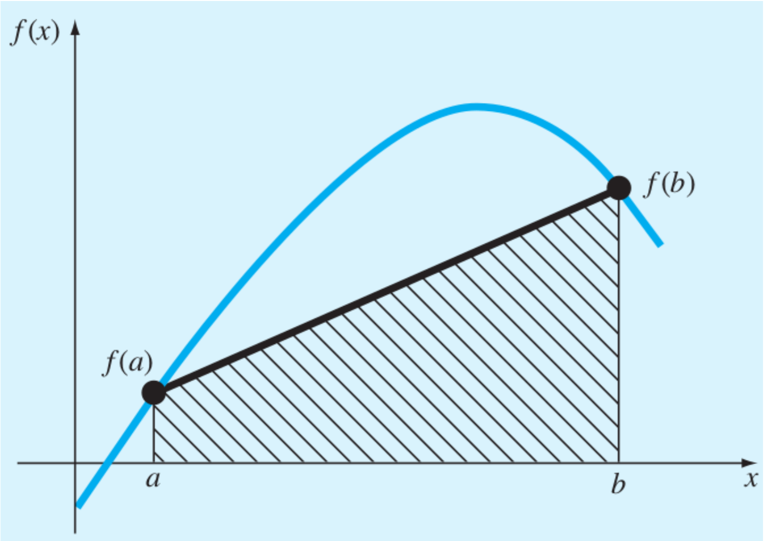
10 Numerical Integration

- A large number of engineering/scientific fields require integration, for example calculating average fluid flow, centres of mass, position of an object using accelerometer data etc.

- Some integrals can be dealt with analytically (as seen in calculus classes), others have no closed-form solution and therefore require approximation.

- When we derived the definite integral in calculus we used the midpoint rule to estimate the area under a curve using rectangles. This method is useful for simple approximations by hand, however we will focus on numerical methods that yield more accurate results.

10.1 Trapezium Rule



- Also known as the Trapezoid or Trapezoidal Rule, this method uses the area of a trapezium to estimate the area under the curve.
- For a single interval [*a*, *b*] we approximate as:

$$\int_a^b f(x)\,dx \approx \frac{1}{2}\left[f(a)+f(b)\right](b-a)$$

- The limitation of this method is demonstrated in the next example.

EXAMPLE 1 Use the trapezium rule to numerically integrate the following function between $0 \le x \le 0.8$.

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

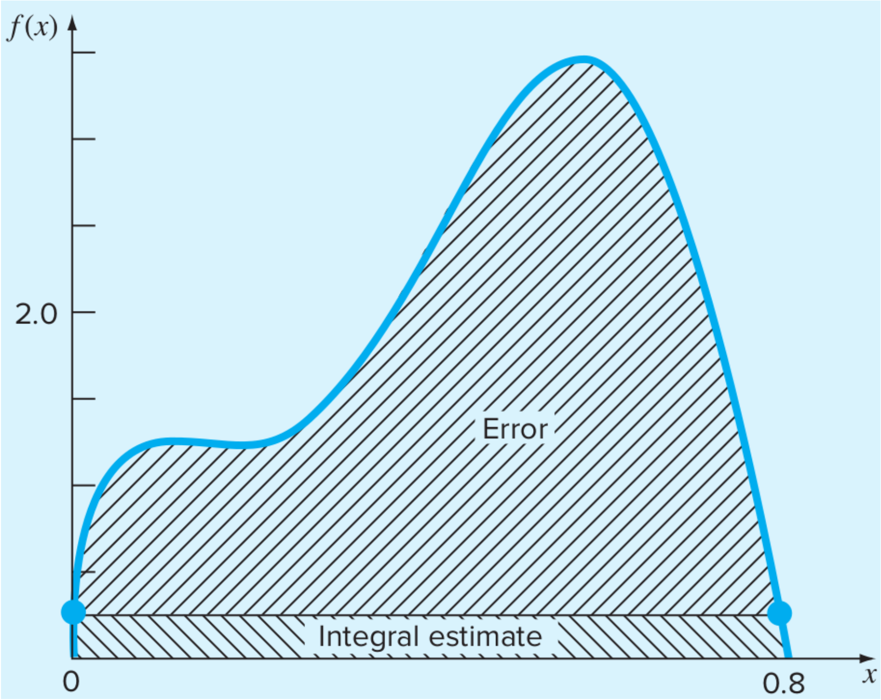
Function values

$$f(0) = 0.2 \qquad f(0.8) = 0.232$$

Trapezium rule

$$I = (0.8 - 0)\,\frac{0.2 + 0.232}{2} = 0.1728$$

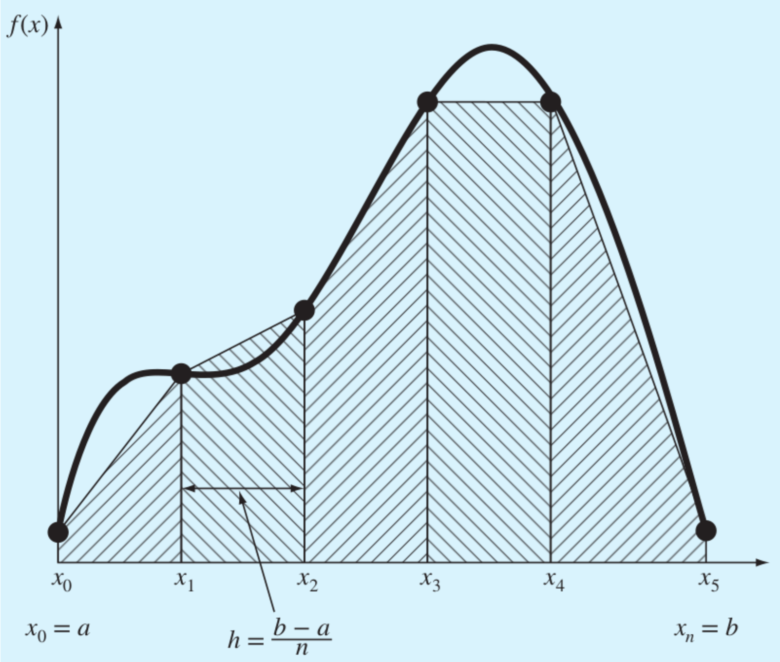
True value = 1.640533



- Notice the large error since evaluating the function at the endpoints was not a fair representation of the function.

Composite Trapezium Rule

- We can improve upon the previous estimate by partitioning the domain into subintervals of width *h* and using the trapezium rule on each part.



$$I = h\frac{f(x_0)+f(x_1)}{2} + h\frac{f(x_1)+f(x_2)}{2} + \cdots + h\frac{f(x_{n-1})+f(x_n)}{2}$$

$$\boxed{= \frac{h}{2}\left[f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)\right]}$$

EXAMPLE 2 Use the composite trapezium rule to perform the same integral as **Example 1** with $n = 2$.

Subinterval width

$$n = 2 \Rightarrow h = (0.8 - 0)/2 = 0.4$$

Function values at subinterval endpoints

$$f(0) = 0.2 \qquad f(0.4) = 2.456 \qquad f(0.8) = 0.232$$

Composite trapezium rule formula

$$I = 0.8\,\frac{0.2 + 2(2.456) + 0.232}{4} = 1.0688$$

- Notice the error decreases for increasing *n*:

n	h	I	ε_t (%)
2	0.4	1.0688	34.9
3	0.2667	1.3695	16.5
4	0.2	1.4848	9.5
5	0.16	1.5399	6.1
6	0.1333	1.5703	4.3
7	0.1143	1.5887	3.2
8	0.1	1.6008	2.4
9	0.0889	1.6091	1.9
10	0.08	1.6150	1.6

Error Estimate for Composite Trapezium Rule

- Let $x_i = a + ih$ then examine the area underneath one of the subintervals $[x_i, x_{i+1}]$:

Integration by parts

$$\int_{x_i}^{x_i+1} f(x)\,dx = \int_0^h f(t+x_i)\,dt = \Big[(t+A)f(t+x_i)\Big]_0^h - \int_0^h (t+A)f'(t+x_i)\,dt$$

$$= \Big[(t+A)f(t+x_i)\Big]_0^h - \left[\left(\frac{(t+A)^2}{2}+B\right)f'(t+x_i)\right]_0^h$$

$$+ \int_0^h \left(\frac{(t+A)^2}{2}+B\right)f''(t+x_i)\,dt,$$

Integration by parts again

- Normally we omit the constants *A* and *B* until the end of integration by parts but here it serves to help us retrieve a formula for the error estimate.

- Now the right-hand side represents the true area of under the curve on the subinterval $[x_i, x_{i+1}]$. Let us choose the first constant such that,

$$\Big[(t+A)f(t+x_i)\Big]_0^h$$

is the trapezium approximation of the area.

- This will mean that the other 2 terms on the right-hand side will correspond with the error.

- Equating the above part with the trapezium area gives:

$$(h+A)f(h+x_i) - Af(x_i) = (f(x_i)+f(x_{i+1}))h/2$$

- Solving this gives $A = -h/2$.

- Now for the other 2 terms which account for the error, let us choose a value of B so that the 2nd term becomes 0 and all of the error is pushed into the last term. The 2nd term is:

$$\left[\left(\frac{(t+A)^2}{2}+B\right)f'(t+x_i)\right]_0^h = \left(\frac{(h/2)^2}{2}+B\right)f'(h+x_i)-\left(\frac{(-h/2)^2}{2}+B\right)f'(x_i)$$

- So if $B = -h^2/8$ the above becomes 0. Substituting this into the 3rd term gives us the error from the trapezium rule on the subinterval:

$$E_T(i) = \int_0^h \left(\frac{(t-h/2)^2}{2}-\frac{h^2}{8}\right)f''(t+x_i)\;dt$$

- So the trapezium rule can be written as:

$$\int_{x_i}^{x_i+1} f(x)\;dx = \frac{h(f(x_i)+f(x_{i+1}))}{2}+\int_0^h\left(\frac{(t-h/2)^2}{2}-\frac{h^2}{8}\right)f''(t+x_i)\;dt$$

- Add up all the errors from each subinterval:

$$
\begin{aligned}
E_T &= E_T(0) + E_T(1) + \cdots + E_T(n-1) \\
&= \int_0^h \left(\frac{(t-h/2)^2}{2} - h^2/8 \right) f''(t+x_0)\, dt \\
&\qquad + \cdots + \\
&\quad \int_0^h \left(\frac{(t-h/2)^2}{2} - h^2/8 \right) f''(t+x_{n-1})\, dt \\
&= \int_0^h \left(\frac{(t-h/2)^2}{2} - h^2/8 \right) \Big(f''(t+x_0) + \cdots + f''(t+x_{n-1}) \Big)\, dt
\end{aligned}
$$

- We also assume that the 2^{nd} derivative of the function is finite. In other words:

$$
|f''(x)| \leq K \text{ for } a \leq x \leq b
$$

- Taking the absolute value of the error then gives:

$$
\begin{aligned}
|E_T| &= \left|\int_0^h \left(\frac{(t-h/2)^2}{2} - \frac{h^2}{8}\right)\Big(f''(t+x_0) + \cdots + f''(t+x_{n-1})\Big)\,dt\right| \\
&\le \int_0^h \left|\left(\frac{(t-h/2)^2}{2} - \frac{h^2}{8}\right)\Big(f''(t+x_0) + \cdots + f''(t+x_{n-1})\Big)\right|\,dt \\
&= \int_0^h \left|\frac{(t-h/2)^2}{2} - \frac{h^2}{8}\right| \left|f''(t+x_0) + \cdots + f''(t+x_{n-1})\right| dt \\
&\le \int_0^h \left|\frac{(t-h/2)^2}{2} - \frac{h^2}{8}\right| \Big(|f''(t+x_0)| + \cdots + |f''(t+x_{n-1})|\Big)\,dt \\
&\le nK \int_0^h \underbrace{\left|\frac{(t-h/2)^2}{2} - \frac{h^2}{8}\right|}\,dt.
\end{aligned}
$$

f*(*t*) = *t*(*t* – *h*)/2 which is negative on 0 ≤ *t* ≤ *h

- Now we can remove the absolute bars and integrate:

$$\int_0^h \left| \frac{(t-h/2)^2}{2} - \frac{h^2}{8} \right| dt = \int_0^h \left(\frac{h^2}{8} - \frac{(t-h/2)^2}{2} \right) dt = \left[\frac{h^2 t}{8} - \frac{(t-h/2)^3}{6} \right]_0^h$$

$$= \left(\frac{h^3}{8} - \frac{(h/2)^3}{6} + \frac{(-h/2)^3}{6} \right) = \frac{h^3}{12}.$$

- So our total error becomes:

$$|E_T| \le \frac{nKh^3}{12} = \frac{K(b-a)^3}{12n^2}$$

where *K* is an upper bound for the 2nd derivative on the interval [*a*, *b*].

- Note that this is only an estimate of the error since we have to choose a value for *K*.

- It is common to use the average value of the 2nd derivative to rewrite the error instead of an upper bound:

$$\bar{f}'' \cong \frac{\sum_{i=1}^{n} f''(\xi_i)}{n}$$

For each ξ_i in the i th subinterval

- We therefore have an approximate error formula as:

$$\boxed{E_a = -\frac{(b-a)^3}{12n^2}\bar{f}''}$$

where the negative sign comes from consideration of the concavity of the function.

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If the function is concave down on a subinterval will the trapezium rule give a positive or negative error?

Positive

Negative

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If the function is concave down is $\bar{f}''(\xi)$ positive or negative (for $a \leq \xi \leq b$)?

Positive

Negative

Tc 0

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EXAMPLE 3 Calculate the approximate error from **Examples 1** & **2** which correspond with the trapezium rule with n = 1 and 2.

2nd derivative

$$f''(x) = -400 + 4{,}050x - 10{,}800x^2 + 8{,}000x^3$$

Average value

$$\bar{f}''(x) = \frac{\int_0^{0.8} (-400 + 4{,}050x - 10{,}800x^2 + 8{,}000x^3)\, dx}{0.8 - 0} = -60$$

Error estimate for n = 1

$$E_a = -\frac{1}{12}(-60)(0.8)^3 = 2.56$$

Error estimate for n = 2

$$E_a = -\frac{0.8^3}{12(2)^2}(-60) = 0.64$$

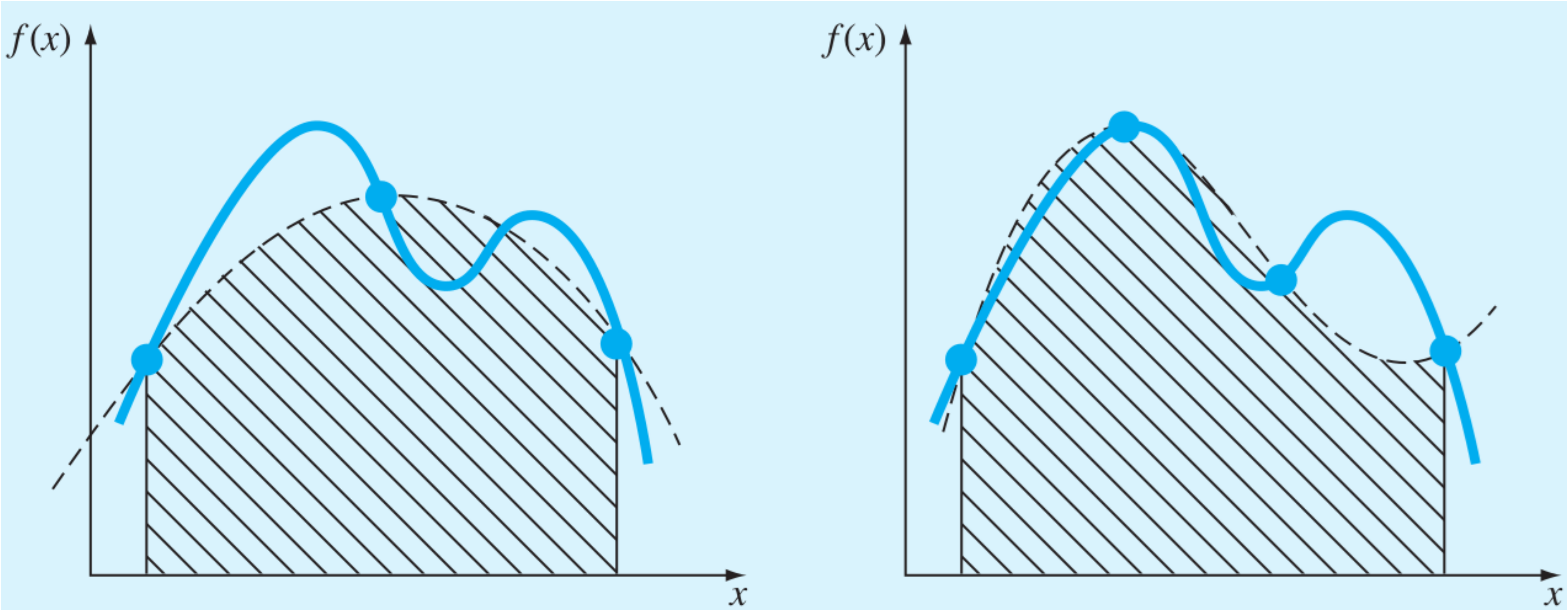
Algorithm for Trapezium Rule

- Partition the domain and calculate the subinterval width, *h*.
- Evaluate the function at the domain endpoints and interior subinterval points.
- Apply the summation formula in an appropriate loop or in vectorised Matlab code:

$$\text{A} = \frac{h}{2}\left[f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)\right]$$

10.2 Simpson's Rules

- Simpson's rules for estimating the area under curves come from either partitioning the domain into 2 parts and approximating the curve with a parabola, or partitioning the domain into 3 parts and approximating the curve with a cubic polynomial.



Simpson's 1/3 Rule

- We select 3 points x_0, x_1 and x_2 from the domain and apply Lagrange interpolation for a quadratic (parabola):

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

- Integrating term by term (with $a = x_0$, $b = x_2$) gives:

$$\boxed{I = (b - a) \frac{f(x_0) + 4f(x_1) + f(x_2)}{6}}$$

- Defining $h = (b - a)/2$ we obtain the **1/3 Rule**:

$$\boxed{I = \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right]}$$

- The approximate error for this rule is given as:

Common to use average value of 4th derivative here

$$E_a = -\frac{1}{90}h^5 f^{(4)}(\xi) = -\frac{(b-a)^5}{2880} f^{(4)}(\xi)$$

for some ξ between *a* and *b*.

EXAMPLE 4 Use Simpson's 1/3 rule with $n = 2$ to integrate the function from **Example 1** between 0 and 0.8 (same as previous examples).

$$n = 2(h = 0.4): \qquad f(0) = 0.2 \qquad f(0.4) = 2.456 \qquad f(0.8) = 0.232$$

$$I = 0.8\,\frac{0.2 + 4(2.456) + 0.232}{6} = 1.367467 \qquad \Bigg| \qquad E_a = -\frac{0.8^5}{2880}(-2400) = 0.2730667$$

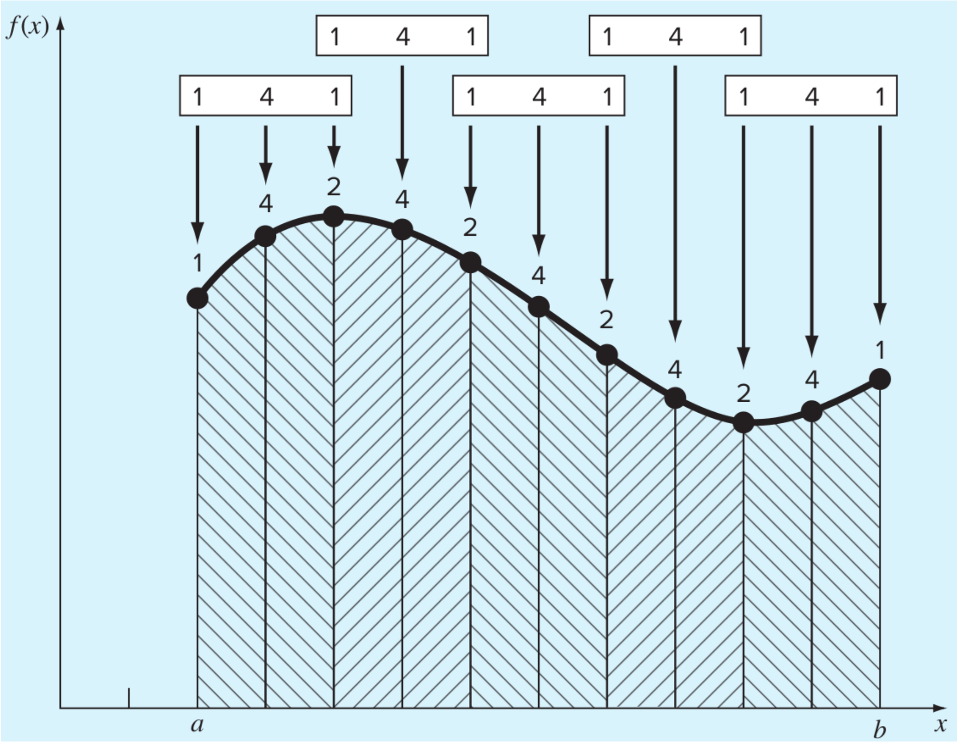
Composite Simpson's 1/3 Rule

- We can partition the domain into more subintervals as long as we choose *n* to be an even number.

$$I = 2h\frac{f(x_0) + 4f(x_1) + f(x_2)}{6} + 2h\frac{f(x_2) + 4f(x_3) + f(x_4)}{6}$$

$$+ \cdots + 2h\frac{f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)}{6}$$

- Remember that *n* corresponds with the number of partitions, not the number of data points (*n* + 1).



- In summation notation we have:

$$\boxed{I = (b-a)\frac{f(x_0) + 4\sum\limits_{i=1,3,5}^{n-1} f(x_i) + 2\sum\limits_{j=2,4,6}^{n-2} f(x_j) + f(x_n)}{3n}}$$

where we used the fact that $h = (b - a)/n$.

- The approximate error is given as:

$$E_a = -\frac{(b-a)^5}{180n^4}\bar{f}^{(4)}$$

Average value of the 4th derivative

EXAMPLE 5 Repeat **Example 4** with $n = 4$.

$$n = 4(h = 0.2): \quad f(0) = 0.2 \quad f(0.2) = 1.288 \quad f(0.4) = 2.456$$

$$f(0.6) = 3.464 \quad f(0.8) = 0.232$$

$$I = 0.8\,\frac{0.2 + 4(1.288 + 3.464) + 2(2.456) + 0.232}{12} = 1.623467$$

$$E_a = -\frac{(0.8)^5}{180(4)^4}(-2400) = 0.017067$$

Algorithm for Simpson's 1/3 Rule

- Partition the domain into an even number of segments.
- Sum the values of the function at odd interval numbers then multiply by 4 (excluding end-points).
- Sum the values of the function at even interval numbers then multiply by 2 (excluding end-points).
- Add the above results to the function values at the endpoints then multiply by $(b - a)/3n$.
- Be careful about the indexes used in Matlab for odd/even interval numbers in the formula.

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Which Matlab code represents Simpson's 1/3 rule if we have defined f as an anonymous function?

```
(b-a)/(3*n)*( f(x(1)) + 4*sum(f(x(2:2:end))) +2*sum(f(x(1:2:end))) + f(x(end)) )
```

```
(b-a)/(3*n)*( f(x(1)) + 4*sum(f(x(2:2:end-2))) +2*sum(f(x(1:2:end-1))) + f(x(end)) )
```

```
(b-a)/(3*n)*( f(x(1)) + 4*sum(f(x(2:2:end-1))) +2*sum(f(x(1:2:end-2))) + f(x(end)) )
```

```
(b-a)/(3*n)*( f(x(1)) + 4*sum(f(x(2:2:end-2))) +2*sum(f(x(3:2:end-1))) + f(x(end)) )
```

```
(b-a)/(3*n)*( f(x(1)) + 4*sum(f(x(2:2:end-1))) +2*sum(f(x(3:2:end-2))) + f(x(end)) )
```

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Simpson's 3/8 Rule

- Used for odd segmented domains (*n* is odd).

- We use 4 points from the domain and fit with a cubic Lagrange polynomial. Integration as before yields:

$$\boxed{I = (b-a)\frac{f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)}{8}}$$

or,

***h* = (*b* – *a*)/3**

$$\boxed{I = \frac{3h}{8}\left[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\right]}$$

- The approximate error is given as:

$$E_a = -\frac{3}{80}h^5 f^{(4)}(\xi) = -\frac{(b-a)^5}{6480} f^{(4)}(\xi)$$

EXAMPLE 6 Use Simpson's 3/8 rule to integrate the function from the previous examples using 4 points in the domain.

4 equispaced points in the domain

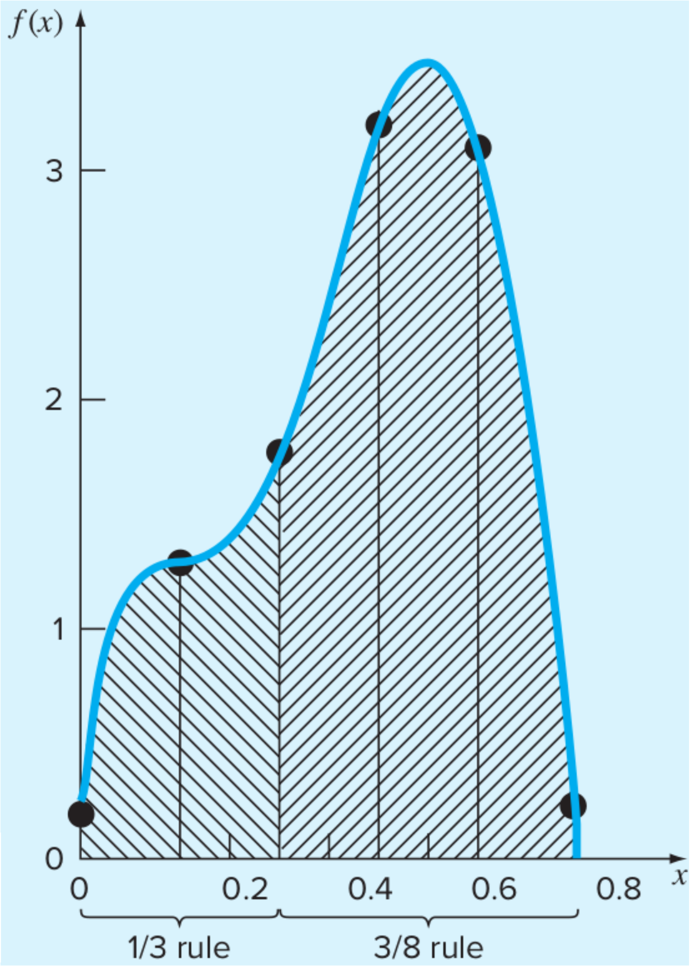
$$f(0) = 0.2 \qquad f(0.2667) = 1.432724$$

$$f(0.5333) = 3.487177 \qquad f(0.8) = 0.232$$

$$I = 0.8\,\frac{0.2 + 3(1.432724 + 3.487177) + 0.232}{8} = 1.51917$$

- We can make a composite 3/8 Simpson's rule formula too however it is more common to combine Simpson's 1/3 rule with the 3/8 rule by splitting the domain segments into an odd and several even parts.

EXAMPLE 7 Use a combination of Simpson's 1/3 rule and 3/8 rule to integrate the function from the previous examples using 5 pieces in the domain.



6 equispaced points

$$f(0) = 0.2 \qquad f(0.16) = 1.296919$$

$$f(0.32) = 1.743393 \qquad f(0.48) = 3.186015$$

$$f(0.64) = 3.181929 \qquad f(0.80) = 0.232$$

1/3 rule

$$I = 0.32\,\frac{0.2 + 4(1.296919) + 1.743393}{6} = 0.3803237$$

3/8 rule

$$I = 0.48\,\frac{1.743393 + 3(3.186015 + 3.181929) + 0.232}{8}$$

$$= 1.264754$$

Total integral $$I = 0.3803237 + 1.264754 = 1.645077$$

10.3 Integration with Uneven Spacing

- It is common in engineering practice to not have a known function that represents our system.

- Instead we often have data measured at certain intervals.

- Quite often the spacing between the data points is not the same so we must be able to integrate in such situations.

- We apply the trapezium method to each subinterval:

$$I = h_1 \frac{f(x_0) + f(x_1)}{2} + h_2 \frac{f(x_1) + f(x_2)}{2} + \cdots + h_n \frac{f(x_{n-1}) + f(x_n)}{2}$$

- Notice the input data (independent variable) must be ***ordered*** for the above formula to work.

EXAMPLE 8 Use the trapezium rule for unequally spaced data points to integrate the following.

x	$f(x)$	x	$f(x)$
0.00	0.200000	0.44	2.842985
0.12	1.309729	0.54	3.507297
0.22	1.305241	0.64	3.181929
0.32	1.743393	0.70	2.363000
0.36	2.074903	0.80	0.232000
0.40	2.456000		

$$I = 0.12\,\frac{0.2 + 1.309729}{2} + 0.10\,\frac{1.309729 + 1.305241}{2}$$

$$+ \cdots + 0.10\,\frac{2.363 + 0.232}{2} = 1.594801$$

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Use the trapezium rule to estimate the distance travelled.

Time (hours)	Velocity (kph)
0	30
0.5	40
2	32
1.5	42

53 km

77 km

90 km

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10.4 Matlab Built-In Functions

- Previously we saw the **diff** function from the symbolic toolbox that allowed us to differentiate symbolic functions.

- We can also use it on vectors to return another vector giving the consecutive differences between the vector elements:

```
>> x = [0 0.3 0.4 0.7 0.55 0.9];
>> diff(x)
ans =
    0.3000    0.1000    0.3000   -0.1500    0.3500
```

- This is useful for checking data when implementing the trapezium rule for unequally spaced data:

```
>> any(diff(x)<0)
ans =
  logical   1
```

Matlab **trapz** and **cumtrapz**

- The **trapz** function implements the trapezium rule for data vectors *x* and *y*.

```
>> x = [0 0.12 0.22 0.32 0.36 0.4 0.44 0.54 0.64 0.7 0.8];
>> y = 0.2 + 25*x - 200*x.^2 + 675*x.^3 - 900*x.^4 + 400*x.^5;
>> trapz(x,y)
ans =
    1.5948
```

- The **cumtrapz** function does the same thing but stores the area underneath the curve between the first data point and the current data point.

```
>> cumtrapz(x,y)
ans =
  Columns 1 through 7
         0    0.0906    0.2213    0.3738    0.4501    0.5407
0.6467
  Columns 8 through 11
    0.9642    1.2987    1.4651    1.5948
```

Matlab **integral**

- We can use the **integral** function to find the definite integral of Matlab functions.

- It's basic usage requires 3 inputs:
  - The function
  - Starting point
  - End point

```
>> f = @(x) 0.2 + 25*x - 200*x.^2 + 675*x.^3 - 900*x.^4
+ 400*x.^5;

>> integral(f,0,0.8)

ans =

    1.6405
```

- We can also pass parameters into functions to integrate:

```
>> f = @(x,a) sin(a*x);
>> integral(@(x) f(x,1),0,pi)
ans =
     2.0000

>> integral(@(x) f(x,2),0,pi)
ans =
   -2.7756e-17

>> integral(@(x) f(x,3),0,pi)
ans =
     0.6667
```

Changing parameter