EAD 115

Numerical Solution of Engineering and Scientific Problems

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Numerical Integration

• Some functions of known form can be integrated analytically
• Others require numerical estimates because the form of the integrand yields no closed form solution
• Sometimes the function may not even be defined by an equation, but rather by a computer program
\[
\int_1^2 x^3 \, dx = \frac{x^4}{4} \bigg|_1^2 = \frac{16}{4} - \frac{1}{4} = \frac{15}{4}
\]

\[
\int_0^{\pi/2} \sin(x) \, dx = -\cos(x) \bigg|_0^{\pi/2}
= -\cos(\pi/2) + \cos(0)
= 0 + 1 = 1
\]

\[
\int_1^4 e^{-x^2} \, dx = ?
\]
The Definite Integral

\[ \int_a^b f(x)\,dx = \lim_{n \to \infty} \sum_{i=0}^{n-1} \left( \frac{b-a}{n} \right) f\left( a + i\frac{b-a}{n} \right) \]

Left and right Riemann sums, and the midpoint rule give definition, not a good computational method. Exact only for constant functions (LR and RR) or linear functions (MR).
\[ \int_{0}^{2} \frac{2 + \cos \left(1 + \frac{x^{3/2}}{2}\right)}{\sqrt{1 + 0.5 \sin x}} \ e^{0.5x} \ dx \]

<table>
<thead>
<tr>
<th>( x )</th>
<th>( f(x) )</th>
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<tbody>
<tr>
<td>0.25</td>
<td>2.599</td>
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<tr>
<td>0.75</td>
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<td>1.945</td>
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<td>1.75</td>
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(c) Discrete points
Continuous function
Example

- \( f(x) = \exp(-x^2) \)
- Use left Riemann sum
- Integrate from 0 to 2
- Exact value is 0.882

<table>
<thead>
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<th>N</th>
<th>Sum</th>
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<tbody>
<tr>
<td>4</td>
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<td>10</td>
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<td>50</td>
<td>0.902</td>
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Trapezoidal Rule

• Simple Riemann sum approximates the function over each interval by a constant function
• We can use linear, quadratic, etc. instead for more accuracy
• Using a linear approximation over each interval results in the trapezoidal rule
Linear and Quadratic Approximations
Linear Approximations over Short Intervals
Closed and Open Rules
Trapezoidal Rule for an Interval

\[ (a, f(a)) \]
\[ (b, f(b)) \]

\[ f_1(x) = f(a) + \frac{f(b) - f(a)}{b - a} (x - a) \]

\[ \int_a^b f_1(x) \, dx = f(a)x + \frac{f(b) - f(a)}{2(b - a)} (x - a)^2 \Bigg|_a^b \]

\[ = f(a)b + \frac{f(b) - f(a)}{2(b - a)} (b - a)^2 - f(a)a \]

\[ = f(a)(b - a) + \frac{f(b) - f(a)}{2} (b - a) \]

\[ = (b - a) \frac{f(b) + f(a)}{2} \]
Trapezoidal Rule for a Subdivided Interval

- Divide the interval \([a, b]\) into \(n\) equal segments, each of width \((b-a)/n\)
- Apply the trapezoidal rule to each segment
- Add up all the results
- This is much more accurate than the simple Riemann sum
\[ h = (b - a) / n \]

\[ x_i = a + ih \quad i = 0, 1, 2, \ldots, n \]

\[ f_i = f(x_i) \]

\[ 0.5h(f_0 + f_1) + 0.5h(f_1 + f_2) + \cdots + 0.5h(f_{n-2} + f_{n-1}) + 0.5h(f_{n-1} + f_n) \]

\[ = 0.5h \left[ f_0 + 2 \sum_{i=1}^{n-1} f_i + f_n \right] = nh \frac{f_0 + 2 \sum_{i=1}^{n-1} f_i + f_n}{2n} \]

\[ = (b - a) \frac{f_0 + 2 \sum_{i=1}^{n-1} f_i + f_n}{2n} = \text{(width)(average height)} \]
$f(x)$

$x_0 = a$

$h = \frac{b - a}{n}$

$x_n = b$
Example

- \( f(x) = \exp(-x^2) \)
- Use trapezoidal rule
- Integrate from 0 to 2
- Exact value is 0.8820814

<table>
<thead>
<tr>
<th>N</th>
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<td>50</td>
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<td>100</td>
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</table>
(a) Single-segment

FUNCTION Trap (h, f0, f1)
    Trap = h * (f0 + f1)/2
END Trap

(b) Multiple-segment

FUNCTION Trapm (h, n, f)
    sum = f0
    DO i = 1, n - 1
        sum = sum + 2 * f_i
    END DO
    sum = sum - f_n
    Trapm = h * sum / 2
END Trapm
Simpson’s Rules
Simpson’s Rules

• Simpson’s rules generalize the trapezoidal rule to use more than two points per interval, so we can use quadratic or cubic models instead of linear.

• We will mainly cover the quadratic model, or Simpson’s 1/3 rule.
Quadratic Interpolation

- For a single interval, we will derive Simpson’s 1/3 rule
- We will need to find the quadratic equation that goes through three points \((x_1, f(x_1)), (x_2, f(x_2)), (x_3, f(x_3))\)
- We will then integrate the quadratic to obtain the estimate of the integral
- This also integrates cubics exactly
\[ f_0 = f(x_0) \quad f_1 = f(x_1) \quad f_2 = f(x_2) \]
\[ h = x_2 - x_1 = x_1 - x_0 \]
\[ \tilde{f}(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f_0 + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f_1 + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f_2 \]
\[ 2h^2 \tilde{f}(x) = (x-x_1)(x-x_2) f_0 - 2(x-x_0)(x-x_2) f_1 + (x-x_0)(x-x_1) f_2 \]
\[ \int_{x_0}^{x_2} \tilde{f}(x) dx = \frac{1}{2h^2} \int_0^{2h} (y-h)(y-2h)f_0 - 2y(y-2h)f_1 + y(y-h)f_2 dy \]
\[ = \frac{h}{3} (f_0 + 4f_1 + f_2) = 2h \frac{f_0 + 4f_1 + f_2}{6} = \text{width/average height} \]
\[ \int_0^{2h} y(y-h)dy = \frac{1}{3} y^3 - \frac{1}{2} hy^2 \bigg|_0^{2h} = \frac{8}{3} h^3 - 2h^3 = \frac{2}{3} h^3 \]
\[ \int_0^{2h} (y-h)(y-2h)dy = \frac{1}{3} y^3 - \frac{3}{2} hy^2 + 2h^2 y \bigg|_0^{2h} = \frac{8}{3} h^3 - 6h^3 + 4h^3 = \frac{2}{3} h^3 \]
\[ -2 \int_0^{2h} y(y-2h)dy = -\frac{2}{3} y^3 + 2hy^2 \bigg|_0^{2h} = -\frac{16}{3} h^3 + 8h^3 = \frac{8}{3} h^3 \]
Simpson’s 1/3 Rule for a Subdivided Interval

- Divide the interval \([a, b]\) into \(n\) equal segments, each of width \((b-a)/n\)
- Apply the Simpson’s 1/3 rule to each pair of segments
- Add up all the results
- This is more accurate than the trapezoidal rule
\[
\frac{h}{3} \left[ f_0 + 4f_1 + f_2 + 4f_3 + f_4 + \cdots + f_{n-4} + 4f_{n-3} + f_{n-2} + 4f_{n-1} + f_n \right]
\]

\[
\frac{h}{3} \left[ f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \cdots + 2f_{n-4} + 4f_{n-3} + 2f_{n-2} + 4f_{n-1} + f_n \right]
\]

\[n = 2m \text{ is even}\]
Example

- \( f(x) = \exp(-x^2) \)
- Use Simpson’s rule
- Integrate from 0 to 2
- Exact value is 0.8820814

<table>
<thead>
<tr>
<th>N</th>
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<tbody>
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<td>0.8820814</td>
</tr>
<tr>
<td>100</td>
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Simpson’s 3/8 Rule

• Uses four points to fit a cubic polynomial
• Is not theoretically more accurate than the 1/3 rule, but can use an odd number of segments
• We can combine this with Simpson’s 1/3 rule if the number of segments is odd
• With 15 intervals (16 points), this is 6 Simpson’s 1/3 rule plus 1 of Simpson’s 3/8 rule
\[ = \frac{3h}{8} \left[ f_0 + 3f_1 + 3f_2 + f_3 \right] \]

\[ = (b - a) \frac{f_0 + 3f_1 + 3f_2 + f_3}{8} \]

\[ = (\text{width})(\text{average height}) \]
(a)
FUNCTION Simp13 (h, f0, f1, f2)
    Simp13 = 2*h*(f0+4*f1+f2) / 6
END Simp13

(b)
FUNCTION Simp38 (h, f0, f1, f2, f3)
    Simp38 = 3*h*(f0+3*(f1+f2)+f3) / 8
END Simp38

(c)
FUNCTION Simp13m (h, n, f)
    sum = f(0)
    DO i = 1, n-2, 2
        sum = sum + 4 * fi + 2 * fi+1
    END DO
    sum = sum + 4 * fn-1 + fn
    Simp13m = h * sum / 3
END Simp13m

(d)
FUNCTION SimpInt(a,b,n,f)
    h = (b - a) / n
    IF n = 1 THEN
        sum = Trap(h,fn-1,fn)
    ELSE
        m = n
        odd = n / 2 - INT(n / 2)
        IF odd > 0 AND n > 1 THEN
            sum = sum + Simp38(h,fn-3,fn-2,fn-1,fn)
            m = n - 3
        END IF
        IF m > 1 THEN
            sum = sum + Simp13m(h,m,f)
        END IF
    END IF
    SimpInt = sum
END SimpInt
Theoretical Errors of Newton-Cotes Methods

- Left and right Riemann integral formulas have errors of $O(h)$. In the case of a linear function, $y = c+dx$ for example, integrated over the interval $[a, b]$, each approximating rectangle is missing a triangular portion whose base is $h$ and whose height is $dh$, and there are $n$ such triangles ($h$ is the length of the interval divided by $n$), so the total error is $ndh^2 / 2 = d(b-a)h/2$, which is proportional to $h$
Improving Left and Right Riemann Sums

• We can eliminate these triangles in two ways
• We can use a central Riemann sum that uses points in the middle of the intervals (open rule). This fits straight lines exactly
• We can use the trapezoidal rule, which also fits straight lines exactly
• Both these have $O(h^2)$ errors
Error in Simpson’s Rule

- The error in Simpson’s 1/3 rule is is $O(h^4)$
- Compare this to left and right Riemann sums with errors at $O(h)$ and the central Riemann sum and trapezoidal rule with errors at $O(h^2)$
- This means that in general Simpson’s rule is more accurate at a given value of $n$
- It also gives information about changes of errors with $n$
Absolute Errors of Three Integration Methods
\( f(x) = \exp(-x^2) \), Integrate from 0 to 2,
Exact value is 0.8820814

<table>
<thead>
<tr>
<th>( N )</th>
<th>( R_L )</th>
<th>Trap</th>
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<td>( 1 \times 10^{-3} )</td>
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<td>( 2 \times 10^{-4} )</td>
<td>( 6 \times 10^{-6} )</td>
</tr>
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