EAD 115

Numerical Solution of Engineering and Scientific Problems

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Is the function available?

• The Newton-Cotes rules we have been looking at need a vector of function values.
• The programs seen previously do not explicitly call a function; rather use a provided grid of values.
• These methods can also be used in the form where a function is called.
• In the case that any value can be called, other methods are available.
(a)

FUNCTION TrapEq (n, a, b)
    h = (b - a) / n
    x = a
    sum = f(x)
    DO i = 1, n - 1
        x = x + h
        sum = sum + 2 * f(x)
    END DO
    sum = sum + f(b)
    TrapEq = (b - a) * sum / (2 * n)
END TrapEq

(b)

FUNCTION SimpEq (n, a, b)
    h = (b - a) / n
    x = a
    sum = f(x)
    DO i = 1, n - 2, 2
        x = x + h
        sum = sum + 4 * f(x)
        x = x + h
        sum = sum + 2 * f(x)
    END DO
    x = x + h
    sum = sum + 4 * f(x)
    sum = sum + f(b)
    SimpEq = (b - a) * sum / (3 * n)
END SimpEq
Fixed Interval vs. Functional Integration

- The Newton-Cotes methods we have been describing all begin with a set of equally spaced function values.
- Sometimes this is all that is available, but we may be able to do better with some variation in the $x$’s.
Richardson Extrapolation

• Given two estimates of an integral with known error properties, it is possible to derive a third estimate that is more accurate

• We will illustrate this with the trapezoidal rule, though the idea applies to any integration method with an error estimate
\[
\int_a^b f(x)dx = I = I(h) + E(h)
\]

For the subdivided interval trapezoidal rule

\[
E(h) = O(h^2) = \frac{b-a}{12} h^2 f''(\xi) \quad \text{for some } \xi \text{ in } [a, b]
\]

\[
I = I(h_1) + E(h_1) = I(h_2) + E(h_2)
\]

\[
\frac{E(h_1)}{E(h_2)} = \frac{h_1^2}{h_2^2} f''(\xi_1) \approx \frac{h_1^2}{h_2^2}
\]

\[
E(h_1) \doteq \frac{h_1^2}{h_2^2} E(h_2)
\]

\[
I(h_1) + \frac{h_1^2}{h_2^2} E(h_2) \doteq I(h_2) + E(h_2)
\]

\[
E(h_2) \doteq \frac{I(h_2) - I(h_1)}{h_1^2/h_2^2 - 1}
\]

\[
I = I(h_2) + E(h_2) = I(h_2) + \frac{I(h_2) - I(h_1)}{h_1^2/h_2^2 - 1} \quad \text{which has error } O(h^4)
\]
For the special case where $h_2 = h_1 / 2$

$$I = I(h_2) + E(h_2) = I(h_2) + \frac{I(h_2) - I(h_1)}{h_1^2 / h_2^2 - 1}$$

$$= I(h_2) + \frac{I(h_2) - I(h_1)}{4 - 1} = I(h_2) + \frac{I(h_2) - I(h_1)}{3}$$

$$= \frac{4}{3} I(h_2) - \frac{1}{3} I(h_1)$$

$$\int_0^2 e^{-x^2} dx = 0.8820814$$

$I(0.2) = 0.8818388$ (n=10)

$I(0.1) = 0.8820204$ (n=20)

$$\frac{4}{3} I(0.1) - \frac{1}{3} I(0.2) = 0.8820810$$

comparable to Simpson's rule with $n = 20$
Repeated Richardson Extrapolation

• With two separate $O(h^2)$ estimates, we can combine them to make an $O(h^4)$ estimate.
• With two separate $O(h^4)$ estimates, we can combine them to make an $O(h^6)$ estimate, etc.
• The weights will be different for these repeated extrapolations.
\[ I_{10}, I_{20}, I_{40} \]

\[ I_{20/10} = \frac{4}{3} I_{20} - \frac{1}{3} I_{10} \]

\[ I_{40/20} = \frac{4}{3} I_{40} - \frac{1}{3} I_{20} \]

\[ I_{40/20/10} = \frac{16}{15} I_{40/20} - \frac{1}{15} I_{20/10} \]

\[ = \frac{64}{45} I_{40} - \frac{20}{45} I_{20} + \frac{1}{45} I_{10} \]
Errors for Richardson Extrapolation from Trapezoidal Rule Estimates

<table>
<thead>
<tr>
<th>n</th>
<th>T</th>
<th>R1</th>
<th>R2</th>
</tr>
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<tr>
<td>10</td>
<td>$2 \times 10^{-4}$</td>
<td></td>
<td>$4 \times 10^{-7}$</td>
</tr>
<tr>
<td>20</td>
<td>$6 \times 10^{-5}$</td>
<td></td>
<td>$5 \times 10^{-11}$</td>
</tr>
<tr>
<td>40</td>
<td>$2 \times 10^{-5}$</td>
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Romberg Integration

- Let $I_{j,k}$ represent an array of estimates of integrals
- $k = 1$ represents trapezoid rules $O(h^2)$
- $k = 2$ represents Richardson extrapolation from pairs of trapezoid rules $O(h^4)$
- $k = 3$ represents Richardson extrapolation from pairs of the previous step at $O(h^6)$, etc.
• If we double the number of points (halve the interval) at each step, then we only need to evaluate the function at the new points
• For example, if the first step uses four intervals, it would involve evaluation at five points, the second one would use eight intervals, evaluated at nine points, only four of which are new

\[ I_{j,k} = \frac{4^{k-1} I_{j+1,k-1} - I_{j,k-1}}{4^{k-1} - 1} \]
FUNCTION Rhomberg (a, b, maxit, es)
    LOCAL I(10, 10)
    n = 1
    I_{1,1} = TrapEq(n, a, b)
    iter = 0
    DO
        iter = iter + 1
        n = 2^iter
        I_{iter+1,1} = TrapEq(n, a, b)
        DO k = 2, iter + 1
            j = 2 + iter - k
            I_{j,k} = (4^{k-1} * I_{j+1,k-1} - I_{j,k-1}) / (4^{k-1} - 1)
        END DO
        ea = ABS((I_{1,iter+1} - I_{1,iter}) / I_{1,iter+1}) * 100
        IF (iter ≥ maxit OR ea ≤ es) EXIT
    END DO
    Rhomberg = I_{1,iter+1}
END Rhomberg
Romberg starting with 2 intervals = 3 points

0.8770373  0.8818124  0.8820824  0.8820814  0.8820814  
0.8806186  0.8820655  0.8820814  0.8820814  0.0000000  
0.8817038  0.8820804  0.8820814  0.0000000  0.0000000  
0.8819862  0.8820813  0.0000000  0.0000000  0.0000000  
0.8820576  0.0000000  0.0000000  0.0000000  0.0000000  

True value is 0.8820814, requires 17 function evaluations to achieve 7-digit accuracy. Simpson’s rule requires 36 function evaluations, and the trapezoidal rule requires 775!
Exact Integration

• The trapezoidal rule integrates a linear function exactly using two points
• Simpson’s 1/3 rule integrates a quadratic (and cubics also) exactly using three points
• It is possible to take n+1 evenly spaced points and choose the weights so that the rule integrates polynomials for degree n exactly (e.g., Simpson’s 3/8 rule)
Gaussian Integration

• Consider a function $f()$ on a closed interval $[a, b]$
• We assume $f()$ is continuous
• We wish to choose $n$ points in $[a, b]$ and weights, so that the weighted sum of the function values at the $n$ points is “optimal”
• Can be chosen to integrate polynomials of degree $2n-1$ exactly
Two interior points can integrate more exactly than two end points.
Two integrals that should be integrated exactly by the trapezoid rule

Method of undetermined coefficients
\[ \int_a^b f(x) \, dx \approx (b - a) \frac{f(a) + f(b)}{2} = c_0 f(a) + c_1 f(b) \quad \text{Trapezoid Rule} \]

\[ f_0(x) = 1 \quad \text{and} \quad f_1(x) = x \quad \text{should be integrated exactly} \]

\[ \int_a^b 1 \, dx = c_0 1 + c_1 1 \]

\[ b - a = h = c_0 + c_1 \]

\[ \int_a^b x \, dx = c_0 a + c_1 b \]

\[ \frac{b^2 - a^2}{2} = c_0 a + c_1 b = c_0 a + (b - a - c_0) b \]

\[ b^2 - a^2 - 2b^2 + 2ab = 2c_0 (a - b) \]

\[ -(a - b)^2 = 2c_0 (a - b) \]

\[ c_0 = \frac{b - a}{2} = c_1 \]
\[
\int_a^b f(x)dx \doteq c_0f_0 + c_1f_1 + c_2f_2
\]
\[
\int_a^b 1dx = b - a = c_0 + c_1 + c_2
\]
\[
\int_a^b xdx = \frac{b^2 - a^2}{2} = c_0a + c_1(a + b)/2 + c_2b
\]
\[
\int_a^b x^2dx = \frac{b^3 - a^3}{3} = c_0a^2 + c_1(a + b)^2/4 + c_2b^2
\]
\[
c_0 = c_2 = (b - a)/6
\]
\[
c_1 = 4(b - a)/6
\]
Simpson's rule
Gauss-Legendre

• Find $n$ points in $[-1, 1]$ and $n$ weights so that the sum of the weighted function values at the chosen points integrates as high a degree polynomial as possible

• $n$ points and $n$ weights means $2n$ coefficients, which is the number in polynomials of degree $2n - 1$

• We find the two-point Gauss-Legendre points and weights for $[-1, 1]$; other intervals follow by substitution
\[
\int_{-1}^{1} f(x)dx = c_0 f(x_0) + c_1 f(x_1)
\]
\[
\int_{-1}^{1} 1dx = 2 = c_0 + c_1
\]
\[
\int_{-1}^{1} xdx = 0 = c_0 x_0 + c_1 x_1
\]
\[
\int_{-1}^{1} x^2 dx = \frac{2}{3} = c_0 x_0^2 + c_1 x_1^2
\]
\[
\int_{-1}^{1} x^3 dx = 0 = c_0 x_0^3 + c_1 x_1^3
\]

\[c_0 = c_1 = 1\]

\[x_0 = \frac{-1}{\sqrt{3}}\]

\[x_1 = \frac{1}{\sqrt{3}}\]
Gaussian Quadrature

• Gauss Legendre is highly accurate with a small number of points
• Suitable for continuous functions on closed intervals
• Gaussian quadrature also comes in other forms: Laguerre, Hermite, Chebychev, etc. for functions with infinite limits of integration, or which are not finite in the interval
• With \( n \) points, Gauss-Laguerre integrates functions exactly that are multiples of \( w(x) = e^{-x} \) by polynomials of degree \( 2n-1 \) exactly.

• \( w(x) \) is called the weight function.

• The weight function for Gauss-Legendre is \( w(x) = 1 \).
\[ w(x) = (1 - x^2)^{-1/2} \quad \text{Chebyshev, first kind} \]
\[ w(x) = (1 - x^2)^{1/2} \quad \text{Chebyshev, second kind} \]
\[ w(x) = e^{-x} \quad \text{Laguerre} \]
\[ w(x) = x^\alpha e^{-x} \quad \text{Generalized Laguerre} \]
\[ w(x) = e^{-x^2} \quad \text{Hermite} \]