Using Numerical Integration

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Numerical Analysis of Engineering Systems

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California State University Northridge

Outline

- Review last lecture
  - Good programming practice
  - Simpson's rule
  - Trapezoid rule
- Selecting the step size for specified error in the numerical integral
  - Using computations for step size h in calculation of numerical integral for h/2
  - Richardson extrapolation and Romberg integration

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Good Programming Practice

- Make programs as general as possible
- Plan your programs before coding
- Use good program structure
  - Logic easy to follow
    - No goto statements
  - Use multiple functions each doing one task
  - Use white space to show structure clearly
- Use comments effectively
- Use meaningful variable names

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Review Numerical Integration

- Numerical integration is used for
  - Functions that have no analytic integral
    - We are able to compute f(x) for any x, but we cannot compute ∫f(x)dx analytically
  - Experimental or tabular data for which no functional relationship exists
- We integrate such functions by using interpolation between tabular data points or computed values of f(x)
  - See example at right

$$I = \int_{1.1}^{2.3} e^{-x^2} dx$$

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Numerical integration formulas

- Simple methods use N+1 evenly-spaced points numbered from 0 to N

Trapezoid rule

$$I = \int_a^b f(x)dx = T + E = h\left[\frac{f_0 + f_N}{2} + \sum_{i=1}^{N-1} f_i\right] + O(h^2)$$

Simpson's rule

$$I = \int_a^b f(x)dx = S + E = \frac{h}{3}\left[f_0 + f_N + 4\sum_{i=1,3,5}^{N-1} f_i + 2\sum_{i=2,4,6}^{N-2} f_i\right] + O(h^4)$$

- Look at example calculations with each of these rules

$$h = \frac{b-a}{N} \qquad x_k = a + kh \qquad f_k = f(x_k)$$

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Apply Trapezoid Rule

$$T = \frac{h}{2}\left[f_0 + f_N + 2\sum_{i=1}^{N-1} f_i\right] \qquad h = \frac{b-a}{N} \qquad x_k = a + kh \qquad f_k = f(x_k)$$

k	x_k	f_k
0	0	1.00
1	0.1	1.10
2	0.2	1.20
3	0.3	1.29
4	0.4	1.37
5	0.5	1.45
6	0.6	1.50

- What are N and h? *N = 6, h = 0.1*
- Write the equation for T using these data

$$T = \frac{0.1}{2}[1.00 + 1.50 + 2(1.10 + 1.20 + 1.29 + 1.37 + 1.45)]$$

T = 0.766

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Apply Simpson's Rule

$$S = \frac{h}{3}\left[f_0 + f_N + 4\sum_{i=1,3,5}^{N-1} f_i + 2\sum_{i=2,4,6}^{N-2} f_i\right] \quad h = \frac{b-a}{N} \quad x_k = a + kh \quad f_k = f(x_k)$$

k	x_k	f_k
0	0	1.00
1	0.1	1.10
2	0.2	1.20
3	0.3	1.29
4	0.4	1.37
5	0.5	1.45
6	0.6	1.50

- What are N and h? ***N = 6*** ***h = 0.1***
- Write the equation for S using these data

$$S = \frac{0.1}{3}[1.00 + 1.50 + 4(1.10 + 1.29 + 1.45) + 2(1.20 + 1.37)]$$

S = 0.7667

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How to Choose h = (b – a)/N

- Numerical integration formulae

$$I = \int_a^b f(x)dx = T + E = h\left[\frac{f_0 + f_N}{2} + \sum_{i=1}^{N-1} f_i\right] + O(h^2)$$

$$I = \int_a^b f(x)dx = S + E = \frac{h}{3}\left[f_0 + f_N + 4\sum_{i=1,3,5}^{N-1} f_i + 2\sum_{i=2,4,6}^{N-2} f_i\right] + O(h^4)$$

- Repeat calculations with different values of N until two values of S (or T) are close enough

$$h = \frac{b-a}{N} \quad x_k = a + kh \quad f_k = f(x_k)$$

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Repeating Calculations

- Look at Trapezoid rule with N = 1, 2, 4, 8, *etc.* steps – what are f(a+kh) sums?

Values in same color are at same x locations

- – L = b – a, h = (b – a)/N = L/N
- – N = 1, sum = f(a)/2 + f(b)/2
- – N = 2, sum = f(a)/2 + f(a+L/2) + f(b)/2
- – N = 4, sum = f(a)/2 + f(a+L/4) + f(a+2L/4) + f(a+3L/4)+ f(b)/2
- – N = 8, sum = f(a)/2 + f(a+L/8) + f(a+2L/8) + f(a+3L/8) + f(a+4L/8) + f(a+5L/8) + f(a+6L/8) + f(a+7L/8) + f(b)/2

$$T = h(sum) \quad (sum) = \frac{f_0 + f_N}{2} + \sum_{i=1}^{N-1} f_i$$

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Repeating Calculations II

- Use sums from previous steps:
  - – N = 1; h = (b – a)/N; sum = [f(a) + f(b)]/2; T = h*(sum)
  - – N = 2; h = (b – a)/N; sum = sum + f(a+h); T = h*(sum)
  - – N = 4; h = (b – a)/N; sum = sum + f(a+h) + f(a+3h); T = h*(sum)
  - – N = 8; h = (b – a)/N; sum = sum + f(a+L/8) + f(a+3L/8) + f(a+5L/8) + f(a+7L/8); T = h*(sum)

$$T = h(sum) \quad (sum) = \frac{f_0 + f_N}{2} + \sum_{i=1}^{N-1} f_i$$

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A General Approach

- The derivation on the next two slides shows that the Trapezoid rule value for step size h, T(h) and the value for step size 2h, T(2h), are related as follows:

$$T(h) = \frac{T(2h)}{2} + h\sum_{k=1,3,5\ldots}^{N-1} f(a+kh)$$

- This equation can be used in code where a conditional loop doubles N, computes the sum shown above, then gets a new T value = oldT/2 + h*sum

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Another Approach II

$$T(2h) = 2h\left[\frac{f(a)+f(b)}{2} + f(a+(1)2h) + f(a+(2)2h) + f(a+(3)2h) + f(a+(4)2h) + \cdots + f(b-2h)\right]$$

$$T(h) = h\left[\frac{f(a)+f(b)}{2} + f(a+h) + f(a+2h) + f(a+3h) + f(a+4h) + \cdots + f(b-2h) + f(b-h)\right]$$

$$\frac{T(2h)}{2} = \frac{2h}{2}\left[\frac{f(a)+f(b)}{2} + f(a+2h) + f(a+4h) + f(a+6h) + f(a+8h) + \cdots + f(b-2h)\right]$$

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Another Approach III

$$T(h) = h\left[\frac{f(a)+f(b)}{2} + f(a+h) + f(a+2h) + f(a+3h) + f(a+4h) + \cdots + f(b-2h) + f(b-h)\right]$$

$$\frac{T(2h)}{2} = \frac{2h}{2}\left[\frac{f(a)+f(b)}{2} + f(a+2h) + f(a+4h) + f(a+6h) + f(a+8h) + \cdots + f(b-2h)\right]$$

$$T(h) - \frac{T(2h)}{2} = h\left[f(a+h) + f(a+3h) + f(a+5h) + \cdots + f(b-h)\right]$$

$$T(h) = \frac{T(2h)}{2} + h\sum_{k=1,3,5\ldots}^{N-1} f(a+kh)$$

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Trapezoid VBA Code

```
converged = false : sum = (f(a) + _
f(b)) : trap = sum*(b - a)/2 : N = 1
Do While not converged
     oldT = trap : N = 2 * N
     h = (b - a) / N : sum = 0
     For k = 1 to N - 1 Step 2
          sum = sum + f(a + k * h)
     Next k
     trap = h * sum + oldT/2
     converged = abs(trap - oldT) <= _
                maxRelErr * abs(trap)
Loop
```

```
Application.Run(f, a + k * h)
```

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Romberg Integration

- Algorithm that simultaneously decreases h (increases N) and increases order of the numerical integration formula
- Based on technique known as Richardson extrapolation
  - This will be covered in next slides
- Romberg integration gives accurate results with automatic setting of step size for desired accuracy

Derivation of Romberg method at end of this presentation

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Richardson Extrapolation

- Uses finite-difference method with two step sizes to get improved accuracy
- Start with E = F(h) + TE = F(h) + O(h^n)
  - E is exact result
  - F(h) is finite difference approximation with step size h
  - Truncation error, TE, is O(h^n)
  - Actually have an infinite series for error

$$TE = \frac{h^n}{n!}\left(\frac{d^n f}{dx^n}\right)_{x=\xi} = \sum_{k=n}^{\infty}\frac{h^n}{n!}\left(\frac{d^n f}{dx^n}\right)_{x=a} = \sum_{k=n}^{\infty} A_k h^k$$

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Richardson Extrapolation II

- Look at evaluating error with two step sizes, h and kh
  - Exact value will not change
  - Create sum to remove first error term

$$E = F(h) + TE = F(h) + \sum_{m=n}^{\infty} A_m h^m = F(h) + A_n h^n + \sum_{m=n+1}^{\infty} A_m h^m$$

$$E = F(kh) + TE = \cdots\cdots = F(kh) + A_n (kh)^n + \sum_{m=n+1}^{\infty} A_m (kh)^m$$

  - Multiply first equation by k^n and subtract it from the second equation to eliminate A_n

$$k^n E - E = k^n F(h) - F(kh) + k^n A_n h^n - A_n (kh)^n + O(h^{n+1})$$

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Richardson Extrapolation III

- Solve equation from previous slide for E

$$k^n E - E = k^n F(h) - F(kh) + O(h^{n+1})$$

$$E = \frac{k^n F(h) - F(kh)}{k^n - 1} + O(h^{n+1}) = RE + O(h^{n+1})$$

- The formula for the Richardson extrapolation, RE, has a higher order of the error
  - Truncation error for RE shown below

$$TE = \frac{k^n \sum_{k=n+1}^{\infty} A_m h^m - \sum_{k=n+1}^{\infty} A_m (kh)^m}{k^n - 1} = \sum_{k=n+1}^{\infty} B_m h^m \qquad B_m = \frac{k^n - k^m}{k^n - 1} A_m$$

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Richardson Extrapolation IV

- What does this mean?

$$E = \frac{k^n F(h) - F(kh)}{k^n - 1} + O\left(h^{n+1}\right) = RE + O\left(h^{n+1}\right)$$

- E is the exact result, F(h) is a finite difference result with step size h
  - If we have two n[th]-order finite difference results, with two step sizes h and kh, we can use this formula to get an improved result with an error order of n + 1

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Richardson Extrapolation V

- Use Richardson extrapolation for dcos(x)/dx at x = 1 and h = 0.1 & h = 0.2
  - What are k and n? ***$k = h_2/h_1 = 2$; n = order = 1***

$$f_i' = \frac{f_{i+1} - f_i}{h} + O\left(h^1\right)$$

$$f_i'(h = 0.1) = \frac{\cos(1.1) - \cos(1)}{0.1} = -0.8670618$$

$$f_i'(h = 0.2) = \frac{\cos(1.2) - \cos(1)}{0.2} = -0.8897228$$

$$RE = \frac{k^n F(h) - F(kh)}{k^n - 1} = \frac{2^1(-0.86706) - -0.88972}{2^1 - 1} = -0.84440093$$

- Extrapolation closer to correct value of $dcos(x)/dx|_{x=1}$ = –sin(1) = –0.8414710

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Romberg Integration

- A technique that starts with a trapezoid rule value for an initial step size, h_{init}
- In a series of iterations, the step size is cut in half for each iteration
- The trapezoid rule is applied to the new step size
- Richardson extrapolation is applied to the trapezoid rule results ***and*** to all previous Richardson extrapolations

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Romberg Integration Notation

- The original trapezoid approximation with h = (b – a)/N_{init} is called T_{00} **N_{init} = 1 or 2**
- As N is doubled we get a sequence of Trapezoid Rule values with N = $2N_{init}$, $4N_{init}$, $8N_{init}$, *etc*. called T_{10}, T_{20}, T_{30}, *etc*.
- After we compute each T_{k0}, we compute Richardson extrapolations $T_{k1}, T_{k2}, \ldots, T_{kk}$
- Continue to double N until we converge with $|T_{kk} - T_{k,k-1}|$ < allowedErr * $|T_{kk}|$

California State University Northridge **T_{k0}= Trapezoid Rule with N=$2^k N_{init}$ steps** 22

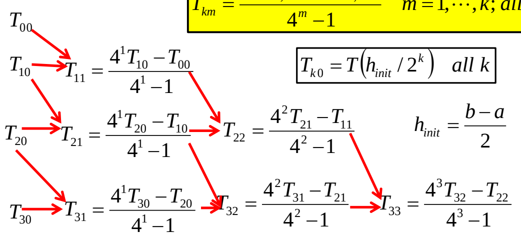
Romberg Integration Structure

- General forms for initial T_{k0} and subsequent T_{km}

$$T_{km} = \frac{4^m T_{k,m-1} - T_{k-1,m-1}}{4^m - 1} \quad m = 1, \cdots, k; \textit{ all } k$$

$$T_{k0} = T\left(h_{init}/2^k\right) \quad \textit{all } k$$

$$h_{init} = \frac{b-a}{2}$$



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Romberg Pseudo Code

```
maxDoubles = 20; err = 1e-10; N = 2;
cvg = false; k = 0; h = (b – a)/2
T00 = h * [f(a) + 2 * f(a+h) + f(b)]/2;
while not cvg and k <= maxDoubles
    k = k + 1; N = 2 * N; h = (b – a)/N
    Loop to sum f(a+mh) for m = 1, N – 1
                                (odd m only)
    Tk0 = Tk-1,0/2 + h * sum
    Loop for m = 1, k to get: Tkm = (4^m Tk,m-1
                   – Tk-1,m-1) / (4^m – 1)
    cvg = abs(Tkk – Tk,k-1) <= err*abs(Tkk)
end while loop
if cvg then ans = Tkk else ans = errorCode
```

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Programming Assignment Six

- Write Romberg integrationcode for in both VBA and MATLAB
  - function I = romberg(f, a, b)
  - Function Romberg(f As String, a As Double, b As Double) As Double
- MATLAB has input function handle for integrand as input to function
- VBA has string with name of VBA function that computes integrand
  - Uses Application.Run procedure

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Romberg Derivation I

- As stated in Rao, page 587, the error of the Trapezoid rule is an infinite series with only even powers of h

$$I = T(h) + \sum_{m=1}^{\infty} A_m h^{2m} = h\left[\frac{f_0 + f_1}{2} + \sum_{k=1}^{N-1} f_k\right] + A_1 h^2 + \sum_{m=2}^{\infty} A_m h^{2m}$$

- Consider two step sizes, h and h/2
  - Apply the Richardson extrapolation formula

$$E = \frac{k^n F(h) - F(kh)}{k^n - 1} + O\left(h^{next}\right) \quad \Rightarrow \quad I = \frac{2^2 T(h/2) - T(h)}{2^2 - 1} + O\left(h^4\right)$$

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Romberg Derivation II

- Define T_{00} as the trapezoid rule value, T(h) and T_{10} as the trapezoid rule value, T(h/2), and T_{11} as the Richardson extrapolation

$$I = T_{11} + O\left(h^4\right) = \frac{2^2 T_{10} - T_{00}}{2^2 - 1} + O\left(h^4\right)$$

- Trapezoid rule for a step size of h/4 is called T_{20}, and Richardson extrapolation with this value is called T_{21}

$$T_{21} = \frac{2^2 T(h/4) - T(h/2)}{2^2 - 1} = \frac{2^2 T_{20} - T_{10}}{2^2 - 1} \qquad I = T_{21} + O\left(h^4\right)$$

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Romberg Derivation III

- The previous slide showed T_{11} and T_{21} as two Richardson extrapolation approximations to the integral
- The error shown as $O(h^4)$ is actually an infinite series with even powers of h
- Each of the Richardson extrapolations is the same calculation starting with two different step sizes
- We can apply Richardson extrapolation to the first set of extrapolated values

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Romberg Derivation IV

- Results now available

$$I = T_{11} + b_2 h^4 + \sum_{m=3}^{\infty} b_m h^{2m} = \frac{2^2 T_{10} - T_{00}}{2^2 - 1} + \sum_{m=2}^{\infty} b_m h^{2m}$$

$$I = T_{21} + b_2\left(\frac{h}{2}\right)^4 + \sum_{m=3}^{\infty} b_m \left(\frac{h}{2}\right)^{2m} = \frac{2^2 T_{20} - T_{10}}{2^2 - 1} + \sum_{m=2}^{\infty} b_m \left(\frac{h}{2}\right)^{2m}$$

- Multiply second equation by 2^4 and subtract the first equation to obtain

$$2^4 I - I = 2^4 T_{21} - T_{11} + 2^4 b_2 \left(\frac{h}{2}\right)^4 - b_2 h^4 + O\left(h^6\right)$$

$$I = \frac{2^4 T_{21} - T_{11}}{2^4 - 1} + O\left(h^6\right) = T_{22} + O\left(h^6\right)$$

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Romberg Derivation V

- What have we done?
  - Started with trapezoid rule calculation with step size h, called T_{00}
  - Did trapezoid rule calculation with step size h/2, called T_{10} and used Richardson extrapolation to get T_{11} from T_{00} and T_{10}
  - Did trapezoid rule calculation with step size h/4, called T_{20} and used two Richardson extrapolations: (1) get T_{21} from T_{10} and T_{20}, and (2) get T_{22} from T_{21} and T_{11}

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Romberg Integration VII

- What is next row in this sequence?

T_{00}

T_{10} $T_{11} = \frac{2^2 T_{10} - T_{00}}{2^2 - 1}$

T_{20} $T_{21} = \frac{2^2 T_{20} - T_{10}}{2^2 - 1}$ $T_{22} = \frac{2^4 T_{21} - T_{11}}{2^4 - 1}$

T_{30} $T_{31} = \frac{2^2 T_{30} - T_{20}}{2^2 - 1}$ $T_{32} = \frac{2^4 T_{31} - T_{21}}{2^4 - 1}$ $T_{33} = \frac{2^6 T_{32} - T_{22}}{2^6 - 1}$

Note that we can replace 2^2, 2^4, 2^6, … by 4^1, 4^2, 4^3, …

- What is(are) the general form(s) for T_{km}?

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Romberg Integration Structure

- General forms for initial T_{k0} and subsequent T_{km}

$$T_{km} = \frac{4^m T_{k,m-1} - T_{k-1,m-1}}{4^m - 1} \quad m = 1, \cdots, k; \; all \; k$$

$$T_{k0} = T\left(h_{init} / 2^k\right) \quad all \; k$$

$$h_{init} = \frac{b-a}{2}$$

T_{00}

T_{10} $T_{11} = \frac{4^1 T_{10} - T_{00}}{4^1 - 1}$

T_{20} $T_{21} = \frac{4^1 T_{20} - T_{10}}{4^1 - 1}$ $T_{22} = \frac{4^2 T_{21} - T_{11}}{4^2 - 1}$

T_{30} $T_{31} = \frac{4^1 T_{30} - T_{20}}{4^1 - 1}$ $T_{32} = \frac{4^2 T_{31} - T_{21}}{4^2 - 1}$ $T_{33} = \frac{4^3 T_{32} - T_{22}}{4^3 - 1}$

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