EAD 115

Numerical Solution of Engineering and Scientific Problems

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Numerical Differentiation

- Previously we learned the forward, backward, and centered difference methods for numerical differentiation
- These use the first-order Taylor-series expansion
- These can be made more accurate by using higher order Taylor series expansions

First-Order Forward Difference

$$f(x+h) = f(x) + f'(x)h + \frac{f''(x_0)}{2}h^2 + O(h^3)$$

$$f'(x)h = f(x+h) - f(x) - \frac{f''(x_0)}{2}h^2 + O(h^3)$$

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{f''(x_0)}{2}h + O(h^2)$$

$$f'(x) = \frac{f(x+h) - f(x)}{h} + O(h)$$

First-Order Second Forward Difference

$$x_0, x_1, \cdots, x_i, x_{i+1}, x_{i+2}, \cdots$$

$$x_{j+1} - x_j = h$$

$$f(x) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2}h^2 + O(h^3)$$

$$f(x_{i+2}) - 2f(x_{i+1}) + f(x_i) = \left(f(x_i) + f'(x_i)2h + \frac{f''(x_i)}{2}4h^2 \right)$$

$$-2\left(f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2}h^2 \right) + f(x_i) + O(h^3)$$

$$= f''(x_i)h^2 + O(h^3)$$

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} + O(h)$$

Second-Order Forward Difference

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f''(x_i)}{2} h + O(h^2)$$

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} + O(h)$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{2h} + O(h^2)$$

$$f'(x) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} + O(h^2)$$

$$\frac{f(x+h) - f(x)}{h} + O(h)$$

$$f(x) = e^{-x^2}$$

$$x = 2$$

$$h = .2$$

$$f(2.0) = 0.0183156389$$

$$f(2.2) = 0.0079070541$$

$$f(2.4) = 0.0031511116$$

$$\frac{f(2.2) - f(2.0)}{.2} = -0.0520429$$

$$\frac{-f(2.4) + 4f(2.2) - 3f(2.0)}{.4} = -.0661745$$

$$f'(x) = -2xe^{-x^2}$$

$$f'(2.0) = -0.07326$$

Numerical error as a function of step size and method

h	E1 O(h)	E2 O(h^2)
0.2	0.021220	0.007088
0.1	0.011658	0.002096
0.05	0.006112	0.000567
0.025	0.003130	0.000147
0.0125	0.001584	0.000037

Factors affecting approximation accuracy

- First or second order method
- Forward or centered difference
- Step size
- All these affect the accuracy of the method

h	Forward 1 O(h)	Forward 2 O(h^2)	Center 1 O(h^2)	Center 2 O(h^4)
0.2	2.12E-02	7.09E-03	4.88E-03	2.96E-05
0.1	1.17E-02	2.10E-03	1.22E-03	1.20E-06
0.05	6.11E-03	5.67E-04	3.05E-04	6.46E-08
0.025	3.13E-03	1.47E-04	7.63E-05	3.87E-09
0.0125	1.58E-03	3.75E-05	1.91E-05	2.39E-10

Richardson Extrapolation

- Just as with numerical integration, estimates with different errors can be combined to reduce the error
- Can be applied iteratively to further reduce the error as in Romberg integration

$$D = D(h) + E(h)$$

$$E(h) = O(h^k)$$

$$D = D(h_1) + E(h_1) = D(h_2) + E(h_2)$$

$$\frac{E(h_1)}{E(h_2)} = \frac{k_1 h_1^2}{k_2 h_2^2} \doteq \frac{h_1^k}{h_2^k}$$

$$E(h_1) \doteq \frac{h_1^k}{h_2^k} E(h_2)$$

$$D(h_1) + \frac{h_1^k}{h_2^k} E(h_2) \doteq D(h_2) + E(h_2)$$

$$E(h_2) \doteq \frac{D(h_2) - D(h_1)}{h_1^2 / h_2^2 - 1}$$

$$D = D(h_2) + E(h_2) \doteq D(h_2) + \frac{D(h_2) - D(h_1)}{h_1^k / h_2^k - 1} \text{ which has error } O(h^{k+2})$$

$$h_2 = h_1 / 2$$

$$h_1^k / h_2^k = 2^k$$

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

$$k = 2$$

$$D(h_2) + \frac{D(h_2) - D(h_1)}{h_1^k / h_2^k - 1} = \frac{4D(h_2) - D(h_1)}{3}$$

Matlab Integration Routines

- The quad function implements adaptive Simpson’s rule
- Adaptive means that some intervals use smaller step sizes than others, and that this depends on the speed of convergence

```
function y=exp2(x)
y=exp(-x.^2)
```

M-File saved as exp2.m

```
>> Q=quad(@exp2,1,2)

Q =


    0.135257216
```

exact answer

0.13525725**58**

The tol parameter controls accuracy

tol	Error
1e-6	4.2 e-8
1e-7	1.8 e-9
1e-7	4.4 e-10