Numerical Differentiation

Ch. 23

Numerical Differentiation

Our previous Taylor Series estimates for derivatives were at Best O(h^2), we will try to improve by retaining more TS terms

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)h^2}{2!} + \frac{f'''(x_i)h^3}{3!} + \frac{f^n(x_i)h^n}{n!} + R_n \quad (1)$$

Solve for *f'(x)*

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

If the f'' term is dropped we get the forward difference approximation

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

the error is of "order h"

Numerical Differentiation

Now, keep the *f''* term and write a forward TS about x_{i+2}

$$f(x_{i+2}) = f(x_i) + f'(x_i)2h + \frac{f''(x_i)4h^2}{2} + \cdots \quad (3)$$

Multiply (1) by 2 and subtract from (3):

$$f(x_{i+2}) = f(x_i) + 2f'(x_i)h + 2f''(x_i)h^2$$

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

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

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

Now substitute (4) into (2)

Numerical Differentiation

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

Simplify,

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

Forward difference method with Error $O(h^2)$

Similar methods can be developed for central and backward differencing in order to obtain higher order accuracy.

See Figure 23.1,23.2 and 23.3 in the text for higher order formulas

Numerical Differentiation
Increasing Accuracy

- Use smaller step size
- Use TS Expansion to obtain higher order formula with more points
- Use 2 derivative estimates to compute a 3rd estimate → Richardson Extrapolation

Effect of Increasing the Number of Segments

Issues:

1. Large number of computations to get high accuracy
2. Accuracy is limited by the computers Precision

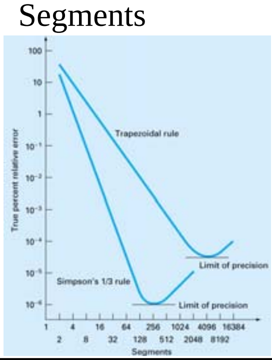


Fig 22.2 Chapra & Canale

We are looking for a higher efficiency method

Richardson Extrapolation

The Idea: Use **TWO** different approximations to some quantity (e.g., a derivative or an integral) to form a **THIRD**, more accurate approximation.

Start by writing an expression for the true value of some quantity as the sum of an approximate value plus the error terms that have been neglected:

$$A = A(h) + Kh^p + O\left(h^{p+1}\right) \qquad (1)$$

Next, rewrite the expression, now using a step size that is **half** as big:

$$A = A\left(\frac{h}{2}\right) + K\frac{h^p}{2^p} + O\left(h^{p+1}\right) \qquad (2)$$

Richardson Extrapolation

In equations (1) and (2), if we neglect the $O(h^{p+1})$ terms we have two equations and two unknowns, *A* and *K*

Remember that *A* is the exact value, while *A(h)* and *A(h/2)* are the approximations computed using those step sizes of *h* and *h/2* respectively, and thus are known

Multiply (2) by 2^p and subtract (1) from that:

$$2^p A = 2^p A\left(\frac{h}{2}\right) + Kh^p + O\left(h^{p+1}\right)$$

$$-A = A(h) + Kh^p + O\left(h^{p+1}\right)$$

this gives:

$$(2^p - 1)A = 2^p A\left(\frac{h}{2}\right) - A(h) + O\left(h^{p+1}\right)$$

Richardson Extrapolation

Finally, solving for *A* gives a new estimate of the exact value that is now $O(h^{p+1})$ accurate:

$$A = \frac{2^p A\left(\frac{h}{2}\right) - A(h)}{(2^p - 1)} + O\left(h^{p+1}\right)$$

For a second order accurate method (*p=2*), this becomes:

$$A = \frac{4A\left(\frac{h}{2}\right) - A(h)}{3} + O\left(h^3\right)$$

Actually, because of term cancellation the Error is $O(h^4)$ for this special case.

Which is the formula the book uses in Eqns. 23.7 & 23.8, BUT those are only correct for second order methods. What would they be for first or third order methods?

Richardson Extrapolation- Integration Example

Suppose we use the Trapezoid rule to integrate:

$f(x)=e^{-x^2}$ from x=0 to x=5

If we use a single application of the Trapezoid Rule:

$$A(h=5)=(5-0)\frac{e^{-25}+e^{0}}{2}=2.5$$

Now using the Trapezoid Rule with 2 intervals:

$$A(h=2.5)=(2.5-0)\frac{e^{-6.25}+e^{0}}{2}+(5-2.5)\frac{e^{-25}+e^{-6.25}}{2}=1.2524+.0024=1.2548$$

Now we can apply the Richardson Extrapolation formula:

$$A=\frac{4A(2.5)-A(5)}{3}=\frac{4(1.2548)-2.5}{3}=.8398$$

Exact answer is .8862 (~5.2% error)

Richardson Extrapolation Differentiation Example

Suppose we use the Forward Differencing to differentiate:

$f(x)=e^{-x^2}$ at $x = 1$ using $h = 0.5$

Single Application of the forward difference method:

$$f'(x_i)=\frac{f(x_{i+1})-f(x_i)}{h}+O(h)=\frac{f(1.5)-f(1)}{0.5}+O(h)=-0.525$$

Now using the Forwdard Diff. and applying Richardson Extrapolation with 2 step sizes $h=1$ and $h=0.5$:

$$A=2A\left(\frac{h}{2}\right)-A(h)=-1.0499-(-0.3496)=-0.70$$

Exact: -0.7358

Relative Errors:

A(h) ~ 52%

A(h/2) ~ 29%

Richardson Extrapolation = 5%

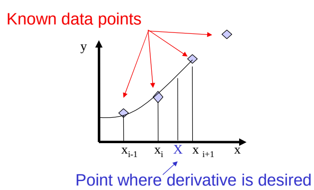
Richardson Extrapolation - Methodology

1. Start with two approximate values using different step sizes
2. Determine Richardson Extrapolation formula based on the order p of the approximate method being used
3. Application of the formula results in a new approximation of accuracy $p+1$
4. This idea can be applied to numerical

Derivatives of Unequally Spaced Data

- Often important for Experimental Data
- 1 option – curve fit the data and take the derivative of the curve.
- Fit a 2nd order Lagrange interpolating polynomial to each set of 3 adjacent data points: (x_{i-1}, x_i, x_{i+1})
- Does NOT require equally spaced data
- Differentiate the Lagrange interpolating polynomial

Fit a 2nd order Lagrange interpolating polynomial



Fit through 3 data points

Derivatives of Unequally Spaced Data

Begin with a 2nd order Lagrange interpolating polynomial:

$$f_2(x) = \frac{(x - x_i)(x - x_{i+1})}{(x_{i-1} - x_i)(x_{i-1} - x_{i+1})} f(x_i) + \frac{(x - x_{i-1})(x - x_{i+1})}{(x_i - x_{i-1})(x_i - x_{i+1})} f(x_i)$$
$$+ \frac{(x - x_{i-1})(x - x_i)}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} f(x_{i+1})$$

Differentiate with respect to *x*:

$$f_2'(x) = \frac{2x - x_i - x_{i+1}}{(x_{i-1} - x_i)(x_{i-1} - x_{i+1})} f(x_{i-1}) + \frac{2x - x_{i-1} - x_{i+1}}{(x_i - x_{i-1})(x_i - x_{i+1})} f(x_i)$$
$$+ \frac{2x - x_{i-1} - x_i}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} f(x_{i+1}) \qquad (*)$$

See Eq. 23.9 & E. 23.3 in text

Derivatives of Unequally Spaced Data

(*) has the same accuracy as Central Differencing if all points are equally spaced ($x = x_i$)

$$f_2^{'}(x) = \frac{2x - x_i - x_{i+1}}{(x_{i-1} - x_i)(x_{i-1} - x_{i+1})} f(x_{i-1}) + \frac{2x - x_{i-1} - x_{i+1}}{(x_i - x_{i-1})(x_i - x_{i+1})} f(x_i)$$

$$+ \frac{2x - x_{i-1} - x_i}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} f(x_{i+1})$$

$$f_2^{'}(x) = \frac{x_i - x_{i+1}}{-h(-2h)} f(x_{i-1}) + \frac{(x_i - x_{i-1}) + (x_i - x_{i+1})}{(h)(-h)} f(x_i) + \frac{x_i - x_{i-1}}{(2h)(h)} f(x_{i+1})$$

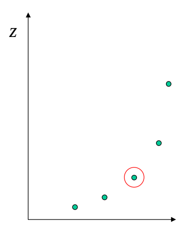
$$f_2^{'}(x) = \frac{-h}{-h(-2h)} f(x_{i-1}) + \frac{h - h}{(h)(-h)} f(x_i) + \frac{h}{(2h)(h)} f(x_{i+1})$$

$$f_2^{'}(x) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h}$$

Central Differencing Formula!

Derivatives of Unequally Spaced Data Wind Speed Example

Calculate the vertical wind shear at 4.3 meters using a 2nd order Lagrange interpolating polynomial.



z (m)	*Wind Speed (m/s)*
1	0.4
2.2	1.2
4.3	3.6
6.1	4.4
10	4.8

Accommodating Data Error in Numerical Differentiation

- Empirical Data include measurement error
- Differentiating data with error will amplify the error
- To overcome this problem:
  - Use least squares regression to fit a smooth curve to data and differentiate the function
  - Low order polynomials are a good choice when relationships between the dependent and independent variables are not known
  - Use a theoretical relationship if one is available

Built in Matlab Differentiation

- Given x and y data one can approximate the derivative using *diff(x)./diff(y)*
  - *diff(x)./diff(y)* = $[x_2 - x_1] / [y_2 - y_1]$
  - *Not a very accurate estimate*