Computational Hydraulics

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Numerical Differentiation and Numerical Integration

Module 5

3 lectures

Contents

- ***Derivatives and integrals***
- ***Integration formulas***
- ***Trapezoidal rule***
- ***Simpson's rule***
- ***Newton's Coats formula***
- ***Gaussian-Quadrature***
- ***Multiple integrals***

Derivatives

Derivatives from difference tables

- We use the divided difference table to estimate values for derivatives. Interpolating polynomial of degree n that fits at points $p_0, p_1, \ldots, p_n$ in terms of divided differences,

$$\begin{aligned} f(x) &= P_n(x) + error \\ &= f[x_0] + f[x_0, x_1](x - x_0) \\ &\quad + f[x_0, x_1, x2](x - x_0)(x - x_1) \\ &\quad + \ldots + f[x_0, x_1, \ldots, x_n] \prod (x - x_i) \\ &\quad + error \end{aligned}$$

- Now we should get a polynomial that approximates the derivative, f'(x), by differentiating it

$$\begin{aligned} P_n{}'(x) &= f[x_0, x_1] + f[x_0, x_1, x_2][(x - x_1) + (x - x_0)] \\ &\quad + \ldots + f[x_0, x_1, \ldots x_n] \sum_{i=0}^{n-1} \frac{(x - x_0)(x - x_1)\ldots(x - x_{n-1})}{(x - x_i)} \end{aligned}$$

Derivatives continued

- To get the error term for the above approximation, we have to differentiate the error term for $P_n(x)$, the error term for $P_n(x)$:

$$Error = (x - x_0)(x - x_1)\ldots(x - x_n)\frac{f^{(n+1)}(\xi)}{(n+1)!}.$$

ξ

- Error of the approximation to f′(x), when $x=x_i$, is

$$Error = \left[\prod_{\substack{j=0 \\ j\neq i}}^{n}(x_i - x_j)\right]\frac{f^{(n+1)}(\xi)}{(n+1)!},$$

ξ in $[x, x_0, x_n]$.

- Error is not zero even when x is a tabulated value, in fact the error of the derivative is less at some x-values between the points

Derivatives continued

Evenly spaced data

- When the data are evenly spaced, we can use a table of function differences to construct the interpolating polynomial.

- We use in terms of: $$s = \frac{(x - x_i)}{h}$$

$$P_n(s) = f_i + s\Delta f_i + \frac{s(s-1)}{2!}\Delta^2 f_i + \frac{s(s-1)(s-2)}{3!}\Delta^3 f_i + \ldots + \prod_{j=0}^{n-1}(s-j)\frac{\Delta^n f_i}{n!} + error;$$

$$Error = \left[\prod_{j=0}^{n}(s-j)\right]\frac{f^{(n+1)}(\xi)}{(n+1)!},$$ ξ in $[x, x_0, x_n]$.

Derivatives continued

- The derivative of $P_n(s)$ should approximate *f'(x)*

$$\frac{d}{dx}P_n(s) = \frac{d}{ds}P_n(s)\frac{ds}{dx}$$

$$= \frac{1}{h}\left[\Delta f_i + \sum_{j=2}^{n}\left\{\sum_{k=0}^{j-1}\prod_{\substack{l=0\\ l\neq k}}^{j-1}(s-l)\right\}\frac{\Delta^j f_i}{j!}\right].$$

- Where

$$\frac{ds}{dx} = \frac{d}{dx}\frac{(x-x_i)}{h} = \frac{1}{h}$$

- When $x=x_i$, $s=0$ $\quad Error = \frac{(-1)^n h^n}{n+1} f^{(n+1)}(\xi),$ ξ in $[x_1, \ldots, x_n]$.

Derivatives continued

Simpler formulas

Forward difference approximation

- For an estimate of $f'(x_i)$, we get

$$f'(x) = \frac{1}{h}[\Delta f_i - \frac{1}{2}\Delta^2 f_i + \frac{1}{3}\Delta^3 f_i - \ldots \pm \frac{1}{n}\Delta^n f_i]_{x=x_i}$$

- With one term, linearly interpolating, using a polynomial of degree 1, we have (error is O(h))

$$f'(x_i) = \frac{1}{h}[\Delta f_i] - \frac{1}{2} h f''(\xi),$$

- With two terms, using a polynomial of degree 2, we have (error is $O(h^2)$)

$$f'(x_i) = \frac{1}{h}\left[\Delta f_i - \frac{1}{2}\Delta^2 f_i\right] + \frac{1}{3} h^2 f^{(3)}(\xi),$$

Derivatives cont…

Central difference approximation

- Assume we use a second degree polynomial that matches the difference table at x_i, x_{i+1} and x_{i+2} but evaluate it for $f'(x_{i+1})$, using s=1, then

$$f'(x_{i+1}) = \frac{1}{h}\left[\Delta f_i + \frac{1}{2}\Delta^2 f_i\right] + O(h^2),$$

- Or in terms of the f - values we can write

$$f'(x_{i+1}) = \frac{1}{h}\left[(f_{i+1} - f_i) + \frac{1}{2}(f_{i+2} - 2f_{i+1} + f_i)\right] + error$$

$$= \frac{1}{h}\frac{f_{i+2} - f_i}{2} + error,$$

$$error = -\frac{1}{6}h^2 f^{(3)}(\xi) = O(h^2)$$

Derivatives cont…

<u>Higher-Order Derivatives</u>

- We can develop formulas for derivatives of higher order based on evenly spaced data
- Difference operator: $\Delta f(x_i) = \Delta f_i = f_{i+1} - f_i$
- Stepping operator : $Ef_i = f_{i+1}$
- Or : $E^n f_i = f_{i+n}$
- Relation between E and Δ: E=1+ Δ
- Differentiation operator: $D(f) = df/dx, D^n(f) = d^n/dx^n(f)$
- Let us start with $f_{i+s} = E^s f_i,$ where $s = (x - x_i)/h$

$$Df_{i+s} = \frac{d}{dx} f(x_{i+s}) = \frac{d}{dx}(E^s f_i)$$

$$= \frac{1}{h}\frac{d}{ds}(E^s f_i) = \frac{1}{h}(\ln E) E^s f_i$$

Derivatives cont…

If s=0, we get

$$D = \frac{1}{h}\ln(1+\Delta)$$

By expanding for ln(1+Δ), we get f'_i and f''_i

$$f_i' = \frac{1}{h}\left(\Delta f_i - \frac{1}{2}\Delta^2 f_i + \frac{1}{3}\Delta^3 f_i - \frac{1}{4}\Delta^4 f_i + \ldots\right),$$

$$f_i'' = \frac{1}{h^2}\left(\Delta^2 f_i - \Delta^3 f_i + \frac{11}{12}\Delta^4 f_i - \frac{5}{6}\Delta^5 f_i + \ldots\right),$$

Divided differences

Central-difference formula

Extrapolation techniques

Second-derivative computations

Richardson extrapolations

Integration formulas

- The strategy for developing integration formula is similar to that for numerical differentiation
- Polynomial is passed through the points defined by the function
- Then integrate this polynomial approximation to the function.
- This allows to integrate a function at known values

Newton-Cotes integration

$$\int_a^b f(x)dx = \int_a^b P_n(x_s)dx$$

The polynomial approximation of f(x) leads to an error given as:

$$Error = \int_a^b \begin{pmatrix} s \\ n+1 \end{pmatrix} h^{n+1} f^{(n+1)}(\xi)dx$$

Newton-Cotes integration formulas

- To develop the Newton-Cotes formulas, change the variable of integration from x to s. Also $dx = hds$
- For any f(x), assume a polynomial $P_n(x_s)$ of degree 1 i.e n=1

$$\int_{x_0}^{x_1} f(x)dx = \int_{x_0}^{x_1} (f_0 + s\Delta f_0)dx$$

$$= h\int_{s=0}^{s=1} (f_0 + s\Delta f_0)ds$$

$$= hf_0 s\Big]_0^1 + h\Delta f_0 \frac{s^2}{2}\Bigg]_0^1 = h(f_0 + \frac{1}{2}\Delta f_0)$$

$$= \frac{h}{2}\left[2f_0 + (f_1 - f_0)\right] = \frac{h}{2}(f_0 + f_1)$$

Newton-Cotes integration formula cont...

- Error in the above integration can be given as

$$Error = \int_{x_0}^{x_1} \frac{s(s-1)}{2} h^2 f''(\xi) dx = h^3 f''(\xi_1) \int_0^1 \frac{s^2 - s}{2} ds$$

$$= h^3 f''(\xi_1) \left(\frac{s^3}{6} - \frac{s^2}{4} \right) \Bigg]_0^1 = -\frac{1}{12} h^3 f''(\xi_1),$$

- Higher degree leads complexity

Newton-Cotes integration formula cont...

- The basic Newton-Cotes formula for n=1,2,3 i.e for linear, quadratic and cubic polynomial approximations respectively are given below:

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}(f_0 + f_1) - \frac{1}{12}h^3 f''(\xi)$$

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}(f_0 + 4f_1 + f_2) - \frac{1}{90}h^5 f^{iv}(\xi),$$

$$\int_{x_0}^{x_3} f(x)dx = \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3) - \frac{3}{80}h^5 f^{iv}(\xi).$$

Trapezoidal and Simpson's rule

Trapezoidal rule-a composite formula

- Approximating *f(x)* on (x_0, x_1) by a straight line

Romberg integration

- Improve accuracy of trapezoidal rule

Simpson's rule

- Newton-Cotes formulas based on quadratic and cubic interpolating polynomials are Simpson's rules
- Quadratic- Simpson's $\frac{1}{3}$ rule
- Cubic- Simpson's $\frac{3}{8}$ rule

Trapezoidal and Simpson's rule cont…

Trapezoidal rule-a composite formula

- The first of the Newton-Cotes formulas, based on approximating *f(x)* on (x_0, x_1) by a straight line, is trapezoidal rule

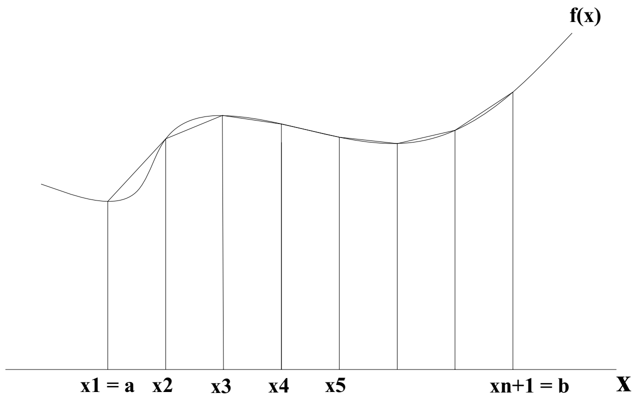
$$\int_{x_i}^{x_{i+1}} f(x)dx = \frac{f(x_i) + f(x_{i+1})}{2}(\Delta x) = \frac{h}{2}(f_i + f_{i+1}),$$

- For [a,b] subdivided into n subintervals of size h,

$$\int_a^b f(x)dx = \sum_{i=1}^{n} \frac{h}{2}(f_i + f_{i+1}) = \frac{h}{2}(f_1 + f_2 + f_2 + f_3 + \ldots + f_n + f_{n+1});$$

$$\int_a^b f(x)dx = \frac{h}{2}(f_1 + 2f_2 + 2f_3 + \ldots + 2f_n + f_{n+1}).$$

Trapezoidal and Simpson's rule cont…



Trapezoidal Rule

Trapezoidal and Simpson's rule cont…

Trapezoidal rule-a composite formula cont…

- Local error $= -\frac{1}{12}h^3 f''(\xi_1),$ $\quad x_0 < \xi_1 < x_1$
- Global error $= -\frac{1}{12}h^3[f''(\xi_1) + f''(\xi_2) + \ldots + f''(\xi_n)],$
- If we assume that f″(x) is continuous on (a,b), there is some value of x in (a,b), say x=ξ, at which the value of the sum in above equation is equal to n.f″(ξ), since nh=b-a, the global error becomes
- Global error

$$= -\frac{1}{12}h^3 n f''(\xi) = \frac{-(b-a)}{12}h^2 f''(\xi) = O(h^2).$$

- The error is of 2nd order in this case

Romberg Integration

- We can improve the accuracy of trapezoidal rule integral by a technique that is similar to Richardson extrapolation, this technique is known as Romberg integration

- Trapezoidal method has an error of $O(h^2)$, we can combine two estimate of the integral that have h-values in a 2:1 ratio by

- Better estimate=more accurate + $\frac{1}{2^n - 1}$(more accurate-less accurate)

Trapezoidal and Simpson's rule

Simpson's rule

- The composite Newton-Cotes formulas based on quadratic and cubic interpolating polynomials are known as Simpson's rule

Quadratic- Simpson's $\frac{1}{3}$ rule

- The second degree Newton-Cotes formula integrates a quadratic over two intervals of equal width, h

$$f(x)dx = \frac{h}{3}\left[f_0 + 4f_1 + f_2\right].$$

- This formula has a local error of $O(h^5)$:

$$Error = -\frac{1}{90}h^5 f^{(4)}(\xi)$$

Trapezoidal and Simpson's rule

Quadratic- Simpson's $\frac{1}{3}$ rule cont...

- For [a,b] subdivided into n (even) subintervals of size h,

$$f(x)dx = \frac{h}{3}\left[f(a) + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \ldots + 4f_{n-1} + f(b)\right].$$

- With an error of

$$Error = -\frac{(b-a)}{180}h^4 f^{(4)}(\xi)$$

- We can see that the error is of 4 th order
- The denominator changes to 180, because we integrate over pairs of panels, meaning that the local rule is applied n/2 times

Trapezoidal and Simpson's rule

Cubic- Simpson's $\frac{3}{8}$ rule

- The composite rule based on fitting four points with a cubic leads to Simpson's $\frac{3}{8}$ rule
- For n=3 from Newton's Cotes formula we get

$$f(x)dx = \frac{3h}{8}\left[f_0 + 3f_1 + 3f_2 + f_3\right].$$

$$Error = -\frac{3}{80}h^5 f^{(4)}(\xi)$$

- The local order of error is same as 1/3 rd rule, except the coefficient is larger

Trapezoidal and Simpson's rule

Cubic- Simpson's $\frac{3}{8}$ rule cont…

- To get the composite rule for [a,b] subdivided into n (n divisible by 3) subintervals of size h,

$$f(x)dx = \frac{3h}{8}[f(a) + 3f_1 + 3f_2 + 2f_3 + 3f_4 + 3f_5 + 2f_6 + \ldots + 2f_{n-3} + 3f_{n-2} + 3f_{n-1} + f(b)]$$

- With an error of

$$Error = -\frac{(b-a)}{80}h^4 f^{(4)}(\xi)$$

Extension of Simpson's rule to Unequally spaced points

- When f(x) is a constant, a straight line, or a second degree polynomial

$$\int_{-\Delta x_1}^{\Delta x_2} f(x)dx = w_1 f_1 + w_2 f_2 + w_3 f_3$$

- The functions *f(x)=1, f(x)=x, f(x)=x²*, are used to establish w_1, w_2, w_3

Gaussian quadrature

- Other formulas based on predetermined evenly spaced x values
- Now unknowns: 3 x-values and 3 weights; total 6 unknowns
- For this a polynomial of degree 5 is needed to interpolate
- These formulas are Gaussian-quadrature formulas
- Applied when f(x) is explicitly known
- Example: a simple case of a two term formula containing four unknown parameters $\int_{-1}^{1} f(t) = af(t_1) + bf(t_2).$
- If we let $x = \frac{(b-a)t+b+a}{2}$ so that $dx = \left(\frac{b-a}{2}\right)dt$ then

$$\int_a^b f(x)dx = \frac{b-a}{2}\int_{-1}^{1} f\left(\frac{(b-a)t+b+a}{2}\right)$$

Multiple integrals

- Weighted sum of certain functional values with one variable held constant
- Add the weighted sum of these sums
- If function known at the nodes of a rectangular grid, we use these values

$$\iint_A f(x,y)\,dA = \int_a^b \left(\int_c^d f(x,y)\,dy \right) dx = \int_c^d \left(\int_a^b f(x,y)\,dx \right) dy$$

- Newton-Cotes formulas are a convenient

$$\int f(x,y)\,dx\,dy = \sum_{j=1}^{m} v_j \sum_{i=1}^{n} w_i f_{ij}$$

$$= \frac{\Delta y}{3} \frac{\Delta x}{2}$$

Multiple integrals

- Double integration by numerical means reduces to a double summation of weighted function values

$$\int_{-1}^{1} f(x)dx = \sum_{i=1}^{n} a_i f(x_i).$$

$$\int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1} f(x,y,z)dxdydz = \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n} a_i a_j a_k f(x_i, y_i, z_k).$$

Assignments

1. Use the Taylor series method to derive expressions for *f'(x)* and *f ''(x)* and their error terms using f-values that precede f_0. (These are called backward-difference formulas.)

2. Evaluate the following integrals by

(i) Gauss method with 6 points

(ii) Trapezoidal rule with 20 points

(iii) Simpson's rule with 10 points

Compare the results. Is it preferable to integrate backwards or forwards?

(a) $\int_0^5 e^{-x^2} dx$ (b) $\int_0^1 x^3 e^{x-1} dx$

Assignments

3. Compute the integral of *f(x)=sin(x)/x* between *x=0* and *x=1* using Simpson's 1/3 rule with h=0.5 and then with h=0.25. from these two results, extrapolate to get a better result. What is the order of the error after the extrapolation? Compare your answer with the true answer.

4. Integrate the following over the region defined by the portion of a unit circle that lies in the first quadrant. Integrate first with respect to *x* holding *y* constant, using *h=0.25*. subdivide the vertical lines into four panels.

$$\iint \cos(x)\sin(2y)\,dx\,dy$$

a. Use the trapezoidal rule
b. Use Simpson's 1/3 rule

Assignments

5. Integrate with varying values of *Δx* and *Δy* using the trapezoidal rule in both directions, and show that the error decreases about in proportion to h^2:

$$\int_0^1 \int_0^1 (x^2 + y^2)\,dx\,dy$$

6. Since Simpson's 1/3 rule is exact when *f(x)* is a cubic, evaluation of the following triple integral should be exact. Confirm by evaluating both numerically and analytically.

$$\int_0^1 \int_0^2 \int_{-1}^0 x^3 y z^2\,dx\,dy\,dz$$