ECE257 Numerical Methods and Scientific Computing

Numerical Integration
Today’s class:

- Numerical Integration
- Newton-Cotes
Numerical Integration

- Numerical technique to solve definite integrals
- Find the area under the curve $f(x)$ from $a$ to $b$

\[ I = \int_{a}^{b} f(x) dx \]

- Another way to put it is that we need to solve the following differential equation

\[ \frac{dy}{dx} = f(x), \quad I = y(b) \text{ and } y(a) = 0 \]
Integration

• Applications
  – Areas of spaces with non-uniform boundaries
  – Means of continuous functions
  – Electric field on a surface area
Numerical Integration

• Where do we use numerical techniques?
  – When you can’t integrate directly
  – When you have a sampling of points representing $f(x)$ as with the experiments results

• Graphical techniques
  – Grid approximation
  – Strip approximation
Graphical Techniques

- Grid approximation
Graphical Techniques

- Strip approximation
Numerical Integration

• Numerical techniques
  – Treat integral as a summation
    \[ I = \int_{a}^{b} f(x)dx = \sum_{i=0}^{n} c_{i}f(x_{i}) \]

• Basic idea is to discretize the continuous function

• The smaller the interval, the more accurate the solution but also at more computational expense
Numerical Integration
Numerical Integration

• Newton-Cotes formulas
  – Approximate function with a series of polynomials that are easy to integrate
    \[ I = \int_{a}^{b} f(x) \, dx \approx \int_{a}^{b} (a_0 + a_1 x + a_1 x^2 + \ldots + a_1 x^n) \, dx \]
  – Zero\(^{th}\) order approximation is equivalent to strip approximation
  – First order approximation is equivalent to trapezoidal approximation
Newton-Cotes Formulas

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Newton-Cotes Formulas

From *Numerical Methods for Engineers*, Chapra and Canale, Copyright © The McGraw-Hill Companies, Inc., John A. Chandy
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Trapezoidal Rule

\[ I = \int_a^b f(x)\,dx \cong \int_a^b f_1(x)\,dx \]

\[ f_1(x) = f(a) + \frac{f(b) - f(a)}{b - a} (x - a) \]

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Trapezoidal Rule

\[ I = \int_a^b \left[ f(a) + \frac{f(b) - f(a)}{b - a} (x - a) \right] dx \]

\[ = f(a) \cdot x + \frac{f(b) - f(a)}{b - a} \left( \frac{x^2}{2} - ax \right) \bigg|_a^b \]

\[ = f(a)(b - a) + \frac{f(b) - f(a)}{b - a} \left( \frac{b^2}{2} - \frac{a^2}{2} - a(b - a) \right) \]

\[ = f(a)(b - a) + \frac{f(b) - f(a)}{b - a} \left( \frac{(b + a)(b - a)}{2} - a(b - a) \right) \]

\[ = f(a)(b - a) + \left( f(b) - f(a) \right) \left( \frac{b - a}{2} \right) \]

\[ = (b - a) \left( \frac{f(b) + f(a)}{2} \right) \]
Trapezoidal Rule

\[ I = (b - a) \left( \frac{f(b) + f(a)}{2} \right) \]

\[ I = (b - a) \times \text{average height} \]

- **Error**

\[ E_t = -\frac{1}{12} f''(\xi)(b - a)^3 \]
Trapezoidal Rule

- Evaluate integral $\int_0^4 xe^{2x} \, dx$

- Analytical solution

$$\int_0^4 xe^{2x} \, dx = \frac{e^{2x}}{4} (2x - 1) \bigg|_0^4 = \frac{e^8}{4} (8 - 1) - \frac{e^0}{4} (0 - 1)$$

$$= 5216.93$$

- Trapezoidal solution

$$\int_0^4 xe^{2x} \, dx = (4 - 0) \frac{f(4) + f(0)}{2} = 4 \frac{4e^8 + 0e^0}{2}$$

$$= 23847.66 \quad \Rightarrow \quad E_t = 18630.74$$
Trapezoidal Rule
Trapezoidal Rule

- Trapezoidal solution
  - To increase accuracy, shorten up the interval

\[
\int_0^4 xe^{2x} \, dx = (2 - 0) \frac{f(2) + f(0)}{2} + (4 - 2) \frac{f(4) + f(2)}{2}
\]

\[
= 2 \frac{2e^4 - 0e^0}{2} + 2 \frac{4e^8 + 2e^4}{2}
\]

\[
= 12142.22 \quad \Rightarrow E_t = 6925.29
\]

\[
\int_0^4 xe^{2x} \, dx = \frac{e^2 + 0e^0}{2} + \frac{2e^4 + e^2}{2} + \frac{3e^6 + 2e^4}{2} + \frac{4e^8 + 3e^6}{2}
\]

\[
= 7288.79 \quad \Rightarrow E_t = 2071.86
\]
Trapezoidal Rule
Trapezoidal Rule

- If you split the interval into $n$ sub-intervals, each sub-interval has a width of $h = \frac{b - a}{n}$

\[
I = \int_{a}^{b} f(x) \, dx = \frac{h}{2} \left[ f(x_0) + f(x_1) + \cdots + f(x_n) \right]
\]

\[
= \frac{h}{2} \left[ \frac{f(x_0) + f(x_n)}{2} + 2 \sum_{i=1}^{n-1} f(x_i) \right]
\]

\[
= \frac{h}{2} \left[ \frac{f(x_0) + f(x_n)}{2} \right]
\]

\[
= (b - a) \frac{f(x_0) + f(x_n)}{2n}
\]

\[
E_a = - \frac{(b - a)^3}{12n^2} \tilde{f}''
\]

average height
Trapezoidal Rule

FUNCTION Trapm (h, n, f)
    sum = f_0
    DO i = 1, n - 1
        sum = sum + 2 * f_i
    END DO
    sum = sum + f_n
    Trapm = h * sum / 2
END Trapm

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Trapezoidal Rule

\texttt{Qtrap(a,b,func)}

\texttt{olds = -INF}

\texttt{for \ j=1 \ to \ JMAX \ do}

\texttt{s = trapm((a-b)/2,j,func)}

\texttt{if \ |s-olds| < \varepsilon_s \ then}

\texttt{return \ s}

\texttt{endif}

\texttt{olds = s}

\texttt{endfor}
Trapezoidal Rule

• More accurate as you increase n
  – Double n and reduce the error by a factor of four

• However, if n is too large, you will start encountering round-off error and the integral solution can diverge
Simpson’s Rules

• Second and third-order polynomial forms of the Newton-Cotes formulas

• Simpson’s 1/3 Rule
  – Use three points on the curve to form a second order polynomial
Simpson’s 1/3-Rule

Approximate the function by a parabola

Approximate the function by a parabola
Simpson’s 1/3-Rule

\[ L(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \]

Let \( x_0 = a, x_2 = b, x_1 = \frac{a+b}{2} \)

\[ h = \frac{b-a}{2}, \quad \xi = \frac{x-x_1}{h}, \quad d\xi = \frac{dx}{h} \]

\[ \begin{align*}
  x = x_0 & \implies \xi = -1 \\
  x = x_1 & \implies \xi = 0 \\
  x = x_2 & \implies \xi = 1
\end{align*} \]

\[ L(\xi) = \frac{\xi(\xi - 1)}{2} f(x_0) + (1 - \xi^2) f(x_1) + \frac{\xi(\xi + 1)}{2} f(x_2) \]
Simpson’s 1/3-Rule

Integrate the Lagrange interpolation

\[
\int_{a}^{b} f(x)\,dx \approx h \int_{-1}^{1} L(\xi)\,d\xi = f(x_{0}) \frac{h}{2} \int_{-1}^{1} \hat{i}(\hat{i} - 1)\,d\hat{i} + f(x_{1}) h \int_{0}^{1} (1 - \hat{i}^{2})\,d\hat{i} + f(x_{2}) \frac{h}{2} \int_{-1}^{1} \hat{i}(\hat{i} + 1)\,d\hat{i}
\]

\[
= f(x_{0}) \frac{h}{2} \left( \frac{\hat{i}^{3}}{3} - \frac{\hat{i}^{2}}{2} \right) \bigg|_{-1}^{1} + f(x_{1}) h(\hat{i} - \frac{\hat{i}^{3}}{3}) \bigg|_{-1}^{1} + f(x_{2}) \frac{h}{2} \left( \frac{\hat{i}^{3}}{3} + \frac{\hat{i}^{2}}{2} \right) \bigg|_{-1}^{1}
\]

\[
\int_{a}^{b} f(x)\,dx = \frac{h}{3} \left[ f(x_{0}) + 4f(x_{1}) + f(x_{2}) \right]
\]
Simpson’s 1/3 Rule

- Error

\[ E_t = -\frac{(b - a)^5}{2880} f^{(4)}(\xi) \]

- Multiple Application

\[ I = \int_a^b f(x) \, dx = (b - a) \frac{f(x_0) + 4 \sum_{i=1,3,5,\ldots}^{n-1} f(x_i) + 2 \sum_{i=2,4,6,\ldots}^{n-2} f(x_i) + f(x_n)}{3n} \]

- n must be even

\[ E_t = -\frac{(b - a)^5}{180n^4} f^{(4)} \]
Simpson’s 1/3 Rule

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Simpson’s 3/8-Rule

Approximate with a cubic polynomial

Approximate with a cubic polynomial

$L(x)$

$f(x)$
Simpson’s 3/8-Rule

\[ L(x) = \frac{(x - x_1)(x - x_2)(x - x_3)}{(x_0 - x_1)(x_0 - x_2)(x_0 - x_3)} f(x_0) \]

\[ + \frac{(x - x_0)(x - x_2)(x - x_3)}{(x_1 - x_0)(x_1 - x_2)(x_1 - x_3)} f(x_1) \]

\[ + \frac{(x - x_0)(x - x_1)(x - x_3)}{(x_2 - x_0)(x_2 - x_1)(x_2 - x_3)} f(x_2) \]

\[ + \frac{(x - x_0)(x - x_1)(x - x_2)}{(x_3 - x_0)(x_3 - x_1)(x_3 - x_2)} f(x_3) \]

\[
\int_a^b f(x) \, dx \approx \int_a^b L(x) \, dx ; \quad h = \frac{b - a}{3}
\]

\[ = \frac{3h}{8} \left[ f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3) \right] \]
Simpson’s 3/8 Rule

• Error

\[ E_t = -\frac{(b - a)^5}{6480} f^{(4)}(\xi) \]

• Multiple Application

\[ I = \int_{a}^{b} f(x)dx = 3(b - a) \frac{f(x_0) + 3 \sum_{i=1,2,4,5\ldots}^{n-1} f(x_i) + 2 \sum_{i=3,6,9\ldots}^{n-3} f(x_i) + f(x_n)}{8n} \]

– n must be a multiple of 3

\[ E_t = -\frac{(b - a)^5}{80n^4} f^{(4)} \]
Simpson’s 3/8 Rule

- Both the cubic and quadratic approximations are of the same order.
- The cubic approximation is slightly more accurate than the quadratic approximation.
- Usually not worth the extra work required.
- Only use the 3/8 rule if you need odd number of segments.
  - Can combine with 1/3 rule on some segments.
Example: Simpson’s Rules

Evaluate the integral \( \int_0^4 xe^{2x} \, dx \)

- **Simpson’s 1/3-Rule**

\[
\int_0^4 xe^{2x} \, dx = (4 - 0) \frac{f(0) + 4f(2) + f(4)}{6} = 4 \frac{0e^0 + 4 \cdot 2 \cdot e^4 + 4e^8}{6}
\]

\[
= 8240.41
\]

\[E_t = 8240.41 - 5216.93 = 3023.48\]

- **Simpson’s 3/8-Rule**

\[
\int_0^4 xe^{2x} \, dx = (4 - 0) \frac{f(0) + 3f\left(\frac{4}{3}\right) + 3f\left(\frac{8}{3}\right) + f(4)}{8} = 4 \frac{0e^0 + 3 \cdot \frac{4}{3} \cdot e^{8/3} + 3 \cdot \frac{8}{3} \cdot e^{16/3} + 4e^8}{8}
\]

\[
= 6819.21
\]

\[E_t = 6819.21 - 5216.93 = 1602.28\]
Simpson’s Rules

```
FUNCTION Simp13m (h, n, f)
    sum = f(0)
    DO i = 1, n - 2, 2
        sum = sum + 4 * f_i + 2 * f_{i+1}
    END DO
    sum = sum + 4 * f_{n-1} + f_n
    Simp13m = h * sum / 3
END Simp13m
```
Simpson’s Rules

Qsimp(a,b,func)

    olds = -INF
    for j=1 to JMAX do
        s = simp13m((a-b)/2,j,func)
        if |s- olds| < $\varepsilon_s$ then
            return s
        endif
        olds = s
    endfor
Simpson’s Rules

Qsimp(a,b,func)
    olds = -INF
    oldst = -INF
    for j=1 to JMAX do
        st = trapm((a-b)/2,j,func)
        s = (4*st-oldst)/3
        if |s-olds| < εs then
            return s
        endif
        olds = s
        oldst = st
    endfor
Integration with unequal segments

- We have until know assumed that each segment is equal
- If we are integrating based on experimental or tabular data, this assumption may not be true
- Newton-Cotes formulas can easily be adapted to accommodate unequal segments
Newton-Cotes Open Formulas

- Sometimes you need to find an integral that extends past the bounds of what you know
- Use the points that you know to extrapolate information past the bounds
- You can use as many points as you have available to extrapolate a line, parabola, cubic, etc.
Trapezoid Rule with Unequal Segments

Evaluate the integral \( I = \int_0^4 xe^{2x} \, dx \)

- \( h_1 = 2, \, h_2 = 1, \, h_3 = 0.5, \, h_4 = 0.5 \)

\[
\int_0^4 xe^{2x} \, dx = \int_0^2 xe^{2x} \, dx + \int_2^3 xe^{2x} \, dx + \int_3^{3.5} xe^{2x} \, dx + \int_{3.5}^4 xe^{2x} \, dx
\]

\[
= 2 \frac{f(0) + f(2)}{2} + \frac{f(2) + f(3)}{2} + 0.5 \frac{f(3) + f(3.5)}{2} + 0.5 \frac{f(3.5) + f(4)}{2}
\]

\[
= 2 \frac{0 e^0 + 2 e^4}{2} + \frac{2 e^4 + 3 e^6}{2} + 0.5 \frac{3 e^6 + 3.5 e^7}{2} + 0.5 \frac{3.5 e^7 + 4 e^8}{2}
\]

\[
= 5971.58
\]

\[
E_t = 5971.58 - 5216.93
\]

\[
= 754.65
\]
Trapezoidal Rule
Simpson’s Rule with Unequal Segments

Evaluate the integral $I = \int_0^4 xe^{2x} \, dx$

- $h_1 = 1.5, \ h_2 = 0.5$

\[
\int_0^4 xe^{2x} \, dx = \int_0^3 xe^{2x} \, dx + \int_3^4 xe^{2x} \, dx \\
= 3 \frac{f(0) + 4f(1.5) + f(3)}{6} + \frac{f(3) + 4f(3.5) + f(4)}{6} \\
= 3 \frac{0e^0 + 4 \cdot 1.5e^3 + 3e^6}{6} + \frac{3e^6 + 4 \cdot 3.5e^7 + 4e^8}{6} \\
= 5413.23
\]

\[
E_t = 5413.23 - 5216.93 \\
= 196.30
\]
Midpoint Rule

Newton-Cotes Open Formula

\[
\int_{a}^{b} f(x) \, dx \approx (b - a) f(x_m)
\]

\[
= (b - a) f\left(\frac{a + b}{2}\right) + \frac{(b - a)^3}{24} f''(\eta)
\]
Two-point Newton-Cotes Open Formula

Approximate by a straight line

$$\int_{a}^{b} f(x)dx \approx \frac{b-a}{2} \left[ f(x_1) + f(x_2) \right] + \frac{(b-a)^3}{108} f''(\eta)$$
Three-point Newton-Cotes Open Formula

Approximate by a parabola

\[
\int_a^b f(x) \, dx \approx \frac{b-a}{3} \left[ 2f(x_1) - f(x_2) + 2f(x_3) \right] + \frac{7(b-a)^5}{23040} f^{(3)}(\eta)
\]
Next Lecture

- Numerical Integration
- Read Chapter 22
- HW4 due 10/21
- HW5 due 10/28