Lecture 18
Scientific and Data Computing I

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Lecture

• Monday – Gaussian Quadrature
• Wednesday – Practicum
Review of Quadrature

• Basic Rules (Newton-Cotes Formulas)
  – Midpoint Rule
  – Trapezoidal Rule
  – Simpson’s Rule

• Composite Quadrature (M segments)

\[
\int_{a}^{b} f(x) \, dx = \sum_{i=0}^{M-1} \int_{x_{i}}^{x_{i+1}} f(x) \, dx
\]
Numerical Integration

• Perspective From Calculus (Riemann Integration):

\[ \int_{x_i}^{x_{i+1}} f(x) \, dx \approx f(c_i)(x_{i+1} - x_i) \]

• Key question: where to select:

\[ c_i \in [x_i, x_{i+1}] \]
Midpoint Rule

• Select the midpoint value:

\[ \int_{x_i}^{x_{i+1}} f(x) \, dx = f(x_i + \frac{h}{2}) h + \mathcal{O}(h^3) \]

\[ h = x_{i+1} - x_i \]
Trapezoidal Rule

- Build a trapezoid:

\[
\int_{x_i}^{x_{i+1}} f(x) \, dx = \frac{h}{2} (f_{i+1} + f_i) - \frac{1}{12} h^3 f''(x_i) + \ldots
\]

\[h = x_{i+1} - x_i\]
Simpson’s Rule

• Build a parabola:

\[
\int_{x_i-1}^{x_{i+1}} f(x)\,dx = \frac{h}{3} (f_{i-1} + 4f_i + f_{i+1}) - \frac{1}{90} h^5 f_i^{\prime\prime\prime\prime}(x_i) + \ldots
\]
Numerical Integration

• Perspective of Interpolation

\[ \int_{x_i}^{x+1} f(x) \, dx \approx \int_{x_i}^{x+1} p(x) \, dx \]

\[ p(x) = \sum_{j=1}^{Q} f(z_j) \ell_j(x) \]
• Perspective of Interpolation

\[
\int_{x_i}^{x+1} \sum_{j=1}^{Q} f(z_j) \ell_j(x) \, dx
\]

\[
\sum_{j=1}^{Q} f(z_j) \int_{x_i}^{x+1} \ell_j(x) \, dx
\]

\[
w_j = \int_{x_i}^{x+1} \ell_j(x) \, dx
\]
Numerical Integration (continued)

• Newton-Cotes (evenly-spaced points)

• Clenshaw-Curtis Quadrature (Chebyshev points)

• Gaussian Quadrature (Gauss points)
Precision

• Example:

\[ \int_{x_i}^{x_{i+1}} f(x) \, dx \approx w_1 f(z_1) + w_2 f(z_2) + \ldots + w_l f(z_l) \]

\[ \int_{x_i}^{x_{i+1}} f(x) \, dx = f(x_i + \frac{h}{2}) h + \frac{1}{24} h^3 f''(\eta) \]
**Definition 6.1.** The *precision* of an integration rule is the largest value of $m$ for which the rule is exact for the functions $f(x) = x^k$, for $k = 0, 1, 2, \ldots, m$.

<table>
<thead>
<tr>
<th>$k$</th>
<th>$f(x)$</th>
<th>$\int_{x_i}^{x_{i+1}} f(x) , dx$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>$h$</td>
</tr>
<tr>
<td>1</td>
<td>$x$</td>
<td>$h \left(x_i + \frac{1}{2} h\right)$</td>
</tr>
<tr>
<td>2</td>
<td>$x^2$</td>
<td>$h \left(x_i^2 + hx_i + \frac{1}{3} h^2\right)$</td>
</tr>
<tr>
<td>3</td>
<td>$x^3$</td>
<td>$h \left(x_i^3 + \frac{3}{2} h x_i^2 + h^2 x_i + \frac{1}{4} h^3\right)$</td>
</tr>
<tr>
<td>4</td>
<td>$x^4$</td>
<td>$h \left(x_i^4 + 2hx_i^3 + 2h^2x_i^2 + h^3 x_i + \frac{1}{5} h^4\right)$</td>
</tr>
<tr>
<td>5</td>
<td>$x^5$</td>
<td>$h \left(x_i^5 + \frac{5}{2} x_i^4 h + \frac{10}{3} x_i^3 h^2 + \frac{5}{2} x_i^2 h^3 + x_i h^4 + \frac{1}{6} h^5\right)$</td>
</tr>
</tbody>
</table>
1-Point Gauss

- 1-Point (Midpoint)

\[
\int_{x_i}^{x_{i+1}} f(x) \, dx \approx w_1 f(z_1)
\]

\[
\int_{x_i}^{x_{i+1}} = w_1 z_1^k
\]
1-Point Gauss (continued)

1. $k = 0$: From previous equation, we required that $\int_{x_i}^{x_{i+1}} dx = w_1$, and from this it follows that

$$h = w_1$$

2. $k = 1$: Putting $f = x$ in previous equation, and using the previous table, it is required that

$$h \left( x_i + \frac{1}{2} h \right) = w_1 z_1$$

Given that $w_1 = h$, we obtain $z_1 = x_i + \frac{1}{2} h$

3. $k = 3$: Using the previous table, it is required that

$$h \left( x_i^2 + hx_i + \frac{1}{3} h^2 \right) = h(x_i + \frac{1}{2} h)^2$$
2-Point Gauss

• **Definition**

\[
\int_{x_i}^{x_{i+1}} f(x) \, dx \approx w_1 f(z_1) + w_2 f(z_2)
\]

\[
\int_{x_i}^{x_{i+1}} x^2 \, dx \approx w_1 z_1^2 + w_2 z_2^2
\]

\[
z_i^{\pm} = x_i + \frac{1}{2}h \pm \frac{1}{2\sqrt{3}}h
\]
Gauss Rules (In General)

- Gauss-Lobatto-Legendre
- Gauss-Radau-Legendre
- Gauss-Gauss-Legendre
For Next Time

• Read Chapter 5 and 6
• Start working on Practicums
• Start working on Homework 4 (due on Thursday)
• No Office Hours This Week Due To Travel