MACM 316 Lecture 29 - (c4p1) Numerical Integration

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Lecture Outline

1.

1 Error Behavior of Simpson's Rule (19.12)

It is important to understand the stability property of **Composite Newton-Cotes** integration techniques.

Assume $f(x_i)$ is approximated by $\tilde{f}(x_i)$:

$$f(x_i) = \tilde{f}(x_i) + e_i \qquad 0 \leq i \leq n.$$

where e_i is the roundoff associated with using $\tilde{f}$ to approximate f. Then, the accumulated roundoff error in the Composite Simpson's Rule is

$$\begin{aligned}|e(h)| &= \left|\frac{h}{3}\left[e_0 + 2\sum_{j=1}^{\frac{n}{2}-1} e_{2j} + 4\sum_{j=1}^{\frac{n}{2}} e_{2j-1} + e_n\right]\right| \\ &\leq \frac{h}{3}\left[|e_0| + 2\sum_{j=1}^{\frac{n}{2}-1} |e_{2j}| + 4\sum_{j=1}^{\frac{n}{2}} |e_{2j-1}| + |e_n|\right]\end{aligned}$$

We have a triangle inequality. Assume all e_j are bounded by $\mathcal{E}$.

$$h = \frac{(b-a)}{n}$$

$$
\begin{aligned}
|e(h)| &\leq \frac{h}{3}\left[\mathcal{E} + 2(\frac{n}{2} - 1)\mathcal{E} + 4\frac{n}{2}\mathcal{E} + \mathcal{E}\right] \\
&= \frac{h}{3}3n\mathcal{E} \\
&= nh\mathcal{E} \\
&= (b-a)\mathcal{E}
\end{aligned}
$$

Which is indepentent of h which implies the procedure is stable as $h \to 0$

2 Romberg Integration

An interesting point concerning the composite Trapezoid Rule:

If $f = \in C^2[a, b]$ then there exists a $\mu \in [a, b]$ such that

$$
\begin{aligned}
\int_a^b f(x)\,dx = \frac{h}{2}\left[f(a) + 2\sum_{j=1}^{h-1} f(x_j) + f(b)\right] - \frac{b-a}{12}h^2 f''(\mu) \\
\text{where } h = \frac{b-1}{n} \\
\text{and } x_j = a + jh
\end{aligned}
$$

Thus the error for the composite Trapezoid Rule is $O(h^2)$. In fact we can be more precise. An application of the Euler-MacLaurin summation formula shows that for sufficiently smooth f,

$$
\begin{aligned}
\text{error} \qquad &= c_1h^2 + c_2h^4 + \cdots + c_mh^{2m} + O(h^{2m+2}) \\
\text{where} \quad c_k &= \text{const} \times \left(f^{(2k-1)}(b) - f^{(2k-1)}(a)\right)
\end{aligned}
$$

This shows us that the Composite Trapezoid Rule is extremely accurate for smooth periodic functions, provided h is small enough.

*Note: The error expansion contains only even powers of h, so eliminating the leading error term improves the accuracy by two additional orders of h.

Notice that we know the form of the error, so we can obtain higher order accuracy by using Richardson Extrapolation. (To give Romberg Integration)

2.1 Richardson Extrapolation to obtain Romberg Integration

We will carry out Composite Trapezoid Rule approximations with

$$m_1 = 1, m_2 = 2, m_3 = 4, \ldots, m_n = 2^{n-1} \text{ intervals..}$$

The values of the step sizes h_k corresponding to m_k are

$$h_k = \frac{(b-1)}{m_k} = \frac{(b-1)}{2^{k-1}}.$$

With this notation, the Composite Trapezoid Rule becomes

$$\int_a^b f(x)\,dx = \frac{h_k}{2}\left[f(a) + 2\left(\sum_{i=1}^{2^{k-1}-1} f(a+ih_k)\right) - \frac{(b-a)}{12}h_k^2 f''(\mu_k)\right].$$

where $\mu_k \in (a,b)$

Let $R_{k,1}$ be the approximation to the integral using $m_k = 2^{k-1}$ intervals. **i.e.**

$$R_{1,1} = \frac{h_1}{2}\left[f(a) + f(b)\right] = \frac{(b-1)}{2}\left[f(a) + f(b)\right]$$

$$\begin{aligned} R_{2,1} &= \frac{h_2}{2}\left[f(a) + f(b) + 2f(a_{h2})\right] \\ &= \frac{(b-a)}{4}\left[f(a) + f(b) + 2f(a + \frac{b-1}{2})\right] \\ &= \frac{1}{2}\left[R_{1,1} + h_1 f(a+h_2)\right] \end{aligned}$$

notice that when h is halved, all the old points at which the function was evaluated appear in the new computation- we can avoid repeating the evaluations.

$$R_{3,1} = \frac{1}{2}\left\{R_{2,1} + h_2\left[f(a+h_3) + f(a+3h_3)\right]\right\}.$$

$$\vdots$$

$$R_{k,1} = \frac{1}{2}\left\{R_{k-1,1} + h_{k-1}\left[\sum_{i=1}^{2^{k-2}} f(a + (2i-1)h_k)\right]\right\}.$$

We can apply this equation to perform the first step of Romberg Integration for

$$\int_0^1 e^{-x}\,dx = 1 - e^{-1} \approx 0.63212.$$

$$\begin{aligned}
R_{1,1} &= \frac{(1-0)}{2}[e^{-0} + e^{-1}] \approx 0.68394 \\
R_{2,1} &= \frac{1}{2}\left[R_{1,1} + \frac{(1-0)}{2}e^{-(0+\frac{1}{2})}\right] = 0.64523 \\
R_{3,1} &= 0.65341 \\
R_{4,1} &= 0.63294
\end{aligned}$$

We can obtain a faster convergence using Richardson Extrapolation: Notice that:

$$\begin{aligned}
\int_a^b f(x)\,dx - R_{h,1} &= \sum_{i=1}^{m} c_i h^{2i} + O(h^{2m+2}) \\
&= c_1 h^2 + \sum_{i=2}^{m} c_i h^{2i} + O(h^{2m+2})
\end{aligned}$$

$$\begin{aligned}
\int_a^b f(x)\,dx - R_{h/2,1} &= \sum_{i=1}^{m} c_i h_{h/2}^{2i} + O(h^{2m+2}) \\
&= \frac{c_1 h^2}{4} + \sum_{i=2}^{m}\left(\frac{c_i h^{2i}}{4^i}\right) + O(h^{2m+2})
\end{aligned}$$

Subtracting the first from 4 times the second gives an $O(h_k^4)$ formula:

$$\int_a^b f(x)\,dx - R_{h,2} = \sum_{i=2}^{m} \frac{c_i}{3}\left(\left(\frac{h^{2i}}{4^i}\right) - h^{2i}\right) + O(h^{2m+2})$$

$$\text{where} \quad R_{h,2} = \frac{R_{h,1} + R_{h/2,1} - R_{h,1}}{3}$$

Of course, this procedure can be repeated to eliminate the $O(h_k^4)$ term from the error. Continuing in this manner, we have an $O(h_k^{2j})$ approximation formula defined by

$$R_{kj} = R_{k,j-1} + \frac{R_{k,j-1} - R_{k-1,j-1}}{4^{j-1} - 1}.$$

Ex. Use Romberg Integration to approximate

$$\int_0^1 e^{-x}\,dx.$$

to 5 significant digits.

	$R_{h,1}$	$R_{h,2}$	$R_{h,3}$	$R_{h,4}$	$R_{h,5}$
$R_{1,j}$	.6839397				
$R_{2,j}$	.6452352	.6723337			
$R_{3,j}$	.6354094	.6321312	.6321209		
$R_{4,j}$	.6329434	.6321214	.6321206	.6321206	
$R_{5,j}$	.6323263	.6321206	.6321206	.6321206	.6321206

A typical stopping criterion is that both

$$|R_{n-1,n-1} - R_{n,n} \text{ and } |R_{n-2,n-2} - R_{n,n}| < \mathcal{E}.$$

for some error tolerance $\mathcal{E}$.
Note that we may not observe the expected convergence acceleration if

- The integrand f is not sufficiently smooth. We need $f \in C^{2k+2}[a,b]$ to generate the k^{th} row of the table.

- The coefficients $c_1, c_2, \ldots$ are very small. This happens for periodic functions if the interval of integration is an integer multiple of the period or for functions with extremely small derivatives at the endpoints of the interval of integration.

3 Adaptive Quadrature

Composative quadrature rules necessitate the use of equally spaced points. This does not take into account that some portions of the curve may have large functional variations that require more attention than other portions of the curve. It is useful to introduce a method that adjusts the step size to be smaller over portions of the curve where a larger functional variation occurs. Thi technique is called adaptive quadrature. We will now discuss an adaptive based on Simpson's Rule. The other composite procedures can be modified in a similar manner.