Adaptive Quadrature

Jingjing Huang

October 31, 2012
Introduction
Motivation
Error Estimation
Adaptive Quadrature
Recall:

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

Partition

\[ a = x_1 < x_2 < \ldots < x_{n+1} = b \]

and denote \( h_i = x_{i+1} - x_i \), then

\[ I(f) = \sum_{i=1}^n l_i \]

where,

\[ l_i = \int_{x_i}^{x_{i+1}} f(x) \, dx \]
**Error In Rectangle Rule**

**Recall:** Taylor expansion \( f(x) \) about the midpoint \( y_i = \frac{x_i + x_{i+1}}{2} \)
(in fact, we can expand it at any points within a small neighborhood, the midpoint is a special case.) :

\[
f(x) = f(y_i) + \sum_{p=1}^{\infty} \frac{(x-y_i)^p}{p!} f^{(p)}(y_i).
\]

Integrate the both sides and notes that

\[
\int_{x_i}^{x_{i+1}} (x - y_i)^p \, dx = \begin{cases} 
\frac{h_i^{p+1}}{(p+1)^{2p}} & \text{if } p \text{ is even} \\
0 & \text{if } p \text{ is odd}
\end{cases}
\]

Why?
**Error In Rectangle Rule**

**Recall:** \( h_i = x_{i+1} - x_i \), then:

\[
\int_{x_i}^{x_{i+1}} f(x) \, dx = h_i f(y_i) + \frac{1}{24} h_i^3 f''(y_i) + \frac{1}{1920} h_i^5 f^{(4)}(y_i) + \cdots
\]

Then

\[
R_i(f) = l_i(f) - \frac{1}{24} h_i^3 f''(y_i) - \frac{1}{1920} h_i^5 f^{(4)}(y_i) + \cdots
\]
Rectangle Rule

Function evaluation: \( n \)
Error in Trapezoid Rule

Recall: $h_i = x_{i+1} - x_i$, then:

$$
\int_{x_i}^{x_{i+1}} f(x) \, dx = h_i \frac{f(x_i) + f(x_{i+1})}{2} - \frac{1}{12} h_i^3 f''(y_i) - \frac{1}{480} h_i^5 f^{(4)}(y_i) + \cdots
$$

Then

$$
T_i(f) = I_i(f) + \frac{1}{12} h_i^3 f''(y_i) + \frac{1}{480} h_i^5 f^{(4)}(y_i) + \cdots
$$
Trapezoid Rule

Function evaluation: \( n + 1 \)
Simpson’s Rule

Recall: the Rectangle Rule and Trapezoid Rule

\[ R_i(f) = I_i(f) - \frac{1}{24} h_i^3 f''(y_i) - \frac{1}{1920} h_i^5 f^{(4)}(y_i) + \cdots \]

\[ T_i(f) = I_i(f) + \frac{1}{12} h_i^3 f''(y_i) + \frac{1}{480} h_i^5 f^{(4)}(y_i) + \cdots \]

Then a more accurate method by combing two together

\[ S_i(f) = \frac{2}{3} R_i(f) + \frac{1}{3} T_i(f) \]

\[ = I_i(f) + \frac{1}{2880} h_i^5 f^{(4)}(y_i) + \cdots \]

\[ \underbrace{\text{Error}} \]
Simpson’s Rule

In a few steps, we can get:

\[ S_i(f) = \frac{2}{3} R_i(f) + \frac{1}{3} T_i(f) \]

\[ = \frac{1}{6} h_i [f(x_i) + 4f(\frac{x_i + x_{i+1}}{2}) + f(x_{i+1})] \]

Function evaluation: \( 2n + 1 \)
Adaptive Quadrature

- What is an adaptive quadrature?

**Definition**

Given a predetermined tolerance $\epsilon$, the algorithm automatically determines the panel size so that the computed approximation $Q$ satisfies

$$|Q - \int_a^b f(x)dx| < \epsilon$$
Adaptive Quadrature using Rectangle Rule

How to determine the tolerance \( \epsilon_i \) in subinterval \( i \)?
Adaptive Quadrature using Rectangle Rule

How to determine the tolerance $\epsilon_i$ in subinterval $i$?
How to determine the tolerance $\epsilon_i$ in subinterval $i$?

$\epsilon_i = \frac{h_i}{b-a} \epsilon$

How to evaluate $\epsilon_i$ in the approximation function?
How to determine the tolerance $\epsilon_i$ in subinterval $i$?

\[ \epsilon_i = \frac{h_i}{b-a} \epsilon \]

How to evaluate $\epsilon_i$ in the approximation function?
Error Estimation in Rectangle Rule

- \( R_i(f) = l_i(f) - \frac{1}{24} h_i^3 f''(y_i) - \frac{1}{1920} h_i^5 f^{(4)}(y_i) + \cdots \), then

\[
R_i(f) - l_i(f) \approx \frac{1}{24} h_i^3 f''(y_i)
\]

When \( h_i \) is small.

- Are we going to calculate \( f''(y_i) \)?
Error Estimation in Rectangle Rule

- \( R_i(f) = I_i(f) - \frac{1}{24} h_i^3 f''(y_i) - \frac{1}{1920} h_i^5 f^{(4)}(y_i) + \cdots \), then

\[
R_i(f) - I_i(f) \approx \frac{1}{24} h_i^3 f''(y_i)
\]

When \( h_i \) is small.

- Are we going to calculate \( f''(y_i) \)?
Error Estimation in Rectangle Rule

- Are we going to calculate $f''(y_i)$?

Error $\approx 1/3$ of deference between two iterations

When $h_i$ is small and $f(x)$ is continuous.

Why?
Error Estimation in Rectangle Rule

Are we going to calculate $f''(y_i)$?

Error $\approx \frac{1}{3}$ of deference between two iterations

When $h_i$ is small and $f(x)$ is continuous.

Why?
Error Estimation in Simpson’s Rule

\[ S_i(f) = l_i(f) + \frac{1}{2880} h_i^5 f^{(4)}(y_i) + \cdots \]

\[ R_i(f) - l_i(f) \approx \frac{1}{2880} h_i^5 f^{(4)}(y_i) \]

Error Estimation

\[ \text{Error} \approx \frac{1}{15} \text{ of deference between two iterations} \]

When \( h_i \) is small and \( f(x) \) is continuous.
Error Estimation in Simpson’s Rule

\[ S_i(f) = I_i(f) + \frac{1}{2880} h_i^5 f^{(4)}(y_i) + \cdots \]

\[ R_i(f) - I_i(f) \approx \frac{1}{2880} h_i^5 f^{(4)}(y_i) \]

Error Estimation

Error \approx \frac{1}{15} of deference between two iterations

When \( h_i \) is small and \( f(x) \) is continuous.
Adaptive Quadrature
Adaptive Quadrature
Adaptive Quadrature
Adaptive Quadrature

Legend
- converged interval
- minimum width interval

Function: [Select Function]
Interval: [Select Interval]
Tolerance: [-2]

Select interval
- Calculate
- Subdivide if necessary

>> Next >>

Reset

Default Interval Selection
- Depth First
- Breadth First

T = 5.552285
M = Q = 0.000000
Adaptive Quadrature

Legend
- converged interval
- minimum width interval

Function: 
Interval: 
Tolerance: $-2$

Select interval
Calculate
Subdivide if necessary

>> Next >>

Default Interval Selection
- Depth First
- Breadth First

$T = 1.552285$
$M = Q = 0.000000$
Adaptive Quadrature
Adaptive Quadrature
Adaptive Quadrature
Adaptive Quadrature
Adaptive Quadrature
Adaptive Quadrature
Adaptive Quadrature
Adaptive Quadrature
But...
Adaptive Quadrature

Legend:
- converged interval
- minimum width interval

Function:
Interval:
Tolerance: $-3$

Select interval:
- Calculate
- Subdivide if necessary

Default Interval Selection:
- Depth First
- Breadth First

$T = \text{value}$
$M = \text{value}$
$|T - M| = \text{value}$

$I = 1.000000$
$Q = 0.000000$
Adaptive Quadrature
Adaptive Quadrature
Adaptive Quadrature
Adaptive Quadrature
Adaptive Quadrature
Adaptive Quadrature
Adaptive Quadrature
Adaptive Quadrature
Adaptive Quadrature
Thanks