Numerical Integration (20 points)

Name: Yuhao Wu
ID Number: 260711365

2018-11-30

Rectangle Rule:

Partition $[a, b]$ into n equal subintervals $[x_i, x_{i+1}], i = 0, 1, 2, \ldots, n$ all with width $h = \frac{b-a}{n}$

The area of the rectangle over $[x_i, x_{i+1}]$ is

$$h \cdot f(x_i) = h \cdot f(a + i \cdot h)$$

So, the **total area** of n rectangle panels is

$$I_R = h \cdot \sum_{i=0}^{n-1} f(a + i \cdot h)$$

Theorem 1. Let f' be continuous on $[a, b]$. Then for some $z \in [a, b]$

$$I - I_R = \frac{1}{2}(b-a) \cdot h \cdot f'(z) = O(h)$$

Proof. First, we show that when $h = b - a$ the results holds, which is to prove that

$$I - I_R = \frac{1}{2}(b-a)^2 \cdot f'(z) = O(h) \tag{1}$$

$$\left[Taylor\ Theorem : f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \ldots + \frac{f^{(n)}(a)}{n!}(x-a)^n + R_n(x) \right]$$

For any $x \in [a, b]$, we do Taylor Expansion at a, then we have:

$$f(x) = f(a) + (x-a)f'(z_x) \quad\ where\ z_x \in [a, b] \tag{2}$$

Then:

$$\begin{aligned}
I - I_R &= \int_a^b f(x)\ dx - f(a) \cdot (b-a) \\
&= \int_a^b f(x)\ dx - \int_a^b f(a)\ dx \quad \text{As } f(a) \text{ is a constant} \\
&= \int_a^b [f(x) - f(a)]\ dx \\
&= \int_a^b (x-a)f'(z_x)\ dx \qquad \text{use equation(2)} \\
&= f'(z) \cdot \int_a^b (x-a)\ dx \quad z \in [a, b] \quad \text{(MVT for integral)} \\
&= \frac{1}{2}(b-a)^2 f'(z)
\end{aligned}$$

Now suppose that $[a, b]$ is divided into n equal subinterval by $x_0, x_1, x_2, \ldots, x_n$ with panel width $h = \dfrac{b-a}{n}$

Applying above results to each of the subinterval $[x_i, x_{i+1}]$, then we have:

$$\int_{x_i}^{x_{i+1}} f(x)\ dx - f(x_i) \cdot h = \frac{1}{2}(x_{i+1} - x_i)^2 f'(z_i) = \frac{1}{2}h^2 \cdot f'(z_i) \quad \text{for some } z_i \in [x_i, x_{i+1}] \tag{3}$$

So, we have

$$\begin{aligned} I - I_R &= \int_a^b f(x)\ dx - h \cdot \sum_{i=0}^{n-1} f(x_i) \\ &= \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} f(x)\ dx - h \cdot \sum_{i=0}^{n-1} f(x_i) \\ &= \sum_{i=0}^{n-1} \frac{1}{2}h^2 \cdot f'(z_i) \\ &= n \cdot \frac{1}{2}h^2 \cdot f'(z) \qquad \text{MVT for sum} \\ &= \frac{1}{2}(b-a)h \cdot f'(z) \end{aligned}$$

□

Midpoint Rule:

The Midpoint Rule:

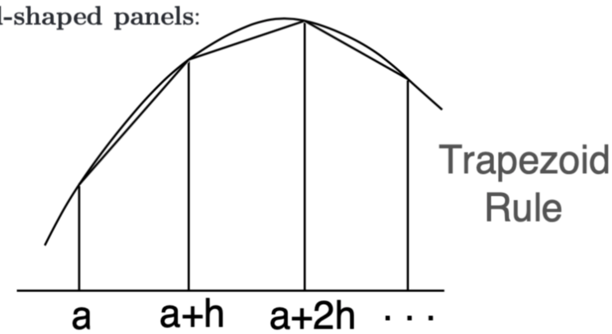
$$I_M = h \sum_{i=0}^{n-1} f\Big[a + (i + \frac{1}{2}h)\Big] \quad \textit{where } h = \frac{b-a}{n}$$

Error Analysis: It can be proven for some $z \in [a, b]$, we have

$$I - I_M = \frac{1}{24}(b-a)h^2 f''(z) = O(h^2)$$

Trapezoid Rule:

Consider **trapezoid-shaped panels**:



For the first panel, the area is $\frac{1}{2} \cdot h \cdot \Big(f(a) + f(a+h)\Big)$

For the second panel, the area is $\frac{1}{2} \cdot h \cdot \Big(f(a+h) + f(a + 2 \cdot h)\Big)$

As all the points are added up twice except for the left-most and right-most points:

$$I_T = \frac{1}{2} \cdot h\Big[f(a) + f(b)\Big] + h \cdot \sum_{i=1}^{n-1} f(a + i \cdot h) \quad \textit{with } h = \frac{b-a}{n}$$

Error Analysis:
It can be shown that for some $z \in [a, b]$

$$I - I_T = -\frac{1}{12}(b-a) \cdot h^2 f''(z) = O(h^2)$$

Recursive Trapezoid Rule:

Suppose that $[a, b]$ is divided into 2^n equal subintervals. Then the trapezoid rule is:

$$I_T(2^n) = \frac{1}{2} \cdot h\Big[f(a) + f(b)\Big] + h \sum_{i=1}^{2^n-1} f(a + i \cdot h) \quad where\ h = \frac{b-a}{2^n}$$

The trapezoid rule for 2^{n-1} equal subintervals is:

$$I_T(2^{n-1}) = \frac{1}{2}\widehat{h} \cdot \Big[f(a) + f(b)\Big] + \widehat{h} \cdot \sum_{i=1}^{2^{n-1}-1} f(a + i \cdot \widehat{h}) \quad where\ \widehat{h} = \frac{b-a}{2^{n-1}} = 2 \cdot h$$

$$\begin{aligned}
I_T(2^n) &= \frac{1}{2}h \cdot \big[f(a) + f(b)\big] + h \sum_{i=1}^{2^n-1} f(a + i \cdot h) + \frac{1}{2} \cdot I_T(2^{n-1}) - \frac{1}{4}\widehat{h} \cdot \Big[f(a) + f(b)\Big] - \frac{1}{2}\widehat{h} \cdot \sum_{i=1}^{2^{n-1}-1} f(a + i \cdot \widehat{h}) \\
&= \frac{1}{2} \cdot I_T(2^{n-1}) + h \sum_{i=1}^{2^n-1} f(a + i \cdot h) - \frac{1}{2}\widehat{h} \cdot \sum_{i=1}^{2^{n-1}-1} f(a + i \cdot \widehat{h}) \\
&= \frac{1}{2} \cdot I_T(2^{n-1}) + h \sum_{i=1}^{2^n-1} f(a + i \cdot h) - h \cdot \sum_{i=1}^{2^{n-1}-1} f(a + i \cdot 2h)
\end{aligned}$$

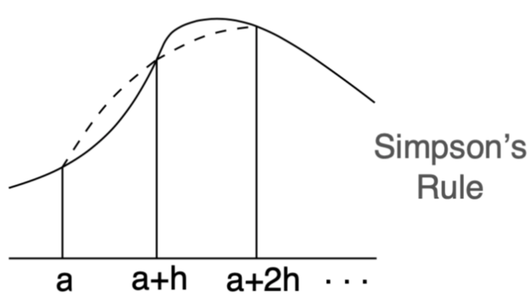
the second term is all the i from 1 to $2^n - 1$ the third term is all the even i from 1 to $2^n - 1$

$$= \frac{1}{2} \cdot I_T(2^{n-1}) + h \cdot \sum_{i=1}^{2^{n-1}} f\Big(a + (2i-1) \cdot h\Big)$$

Why we need Recursive:

- After computing $I_T(2^{n-1})$, we can compute $I_T(2^n)$ by recursive formula without reevaluating f at some old points
- We can use the recursive formula to determine how many iterations we need by $|I_T(2^n) - I_T(2^{n-1})| < \delta$

Simpson's Rule:



There are an even number of panels with width $h = \dfrac{b-a}{n}$.

The top boundary of the first pair of panels is the quadratic which interpolates $(a, f(a)), (a+h, f(a+h)), (a+2h, f(a+2h))$.
The next interpolates $(a+2h, f(a+2h)), (a+3h, f(a+3h)), (a+4h, f(a+4h))$, and so on.

The area of the first 2 panels can be shown to be:

$$\frac{h}{3}\Big[f(a) + 4f(a+h) + f(a+2h)\Big]$$

. For the total area, we sum them up:

$$\begin{aligned}
&\frac{h}{3}\Big[f(a) + 4f(a+h) + f(a+2h)\Big] \\
&\frac{h}{3}\Big[f(a+2h) + 4f(a+3h) + f(a+4h)\Big] \\
&\vdots \\
&\frac{h}{3}\Big[f(b-2h) + 4f(b-h) + f(b)\Big]
\end{aligned}$$

Then we have **Simpson's Rule:**

$$I_S = \frac{h}{3}\Bigg[f(a) + 4\cdot f(a+h) + 2\cdot f(a+2h) + 4f(a+3h) + 2f(a+4h) + \ldots + f(b)\Bigg]$$

As it is divided into $n = 2k$ subintervals, we can rewrite it as:

$$I_S = \frac{h}{3}\Bigg[f(a) + f(b) + 4\cdot\sum_{i=0}^{k-1} f\Big(a + (2i+1)\cdot h\Big) + 2\cdot\sum_{i=1}^{k-1} f\Big(a + 2i\cdot h\Big)\Bigg]$$

Error Analysis:
It can be shown for some $z \in [a, b]$:

$$I - I_S = -\frac{1}{180}\cdot(b-a)\cdot h^4 \cdot f^{(4)}(z) = O(h^4)$$

Question:
What is the highest degree polynomial for which the rule is **exact** in general?

> The highest degree is 3.
> As for polynomial with degree 3, $f^{(4)}(z)$ is always 0, which tells us the error is always 0.

Adaptive Method:

Question: Why do we need Adaptive Method?

A function may vary rapidly on some parts of the interval $[a, b]$, but vary little on other parts. It is not very efficient to use the same panel width h everywhere on $[a, b]$. But on the other hand, we don't know in advance on which part of the integral f varies rapidly. So, we need an adaptive integration method.

Basic Idea:

The basic idea is we divide $[a, b]$ into 2 subintervals and then decide whether each of them is to be divided into more subintervals. This procedure is continued until some specified accuracy is obtained throughout the whole interval $[a, b]$.

Basic Framework:

Algorithm 1 Adaptive Method:

Input: $f(x) \quad a, b, \quad$ the tolerance $\delta, \ldots$

Compute the integral from a and b in two ways
call the values I_1 and I_2 separately (Assume I_2 is better than I_1)
Estimate the error in I_2 based on $|I_2 - I_1|$

if $|$ the Estimated Error $| \leq \delta$ **then**
  $numI = I_2 +$ the Estimated Error
else
  $c = \dfrac{a+b}{2}$
  $numI = adapt(f, a, c, \dfrac{\delta}{2}, \ldots) + adapt(f, c, b, \dfrac{\delta}{2}, \ldots)$
end if

Gaussian Quadrature Rules:

Unlike previous integration rules which choose equally spaced nodes for evaluation, Gaussian Quadrature rules choose the nodes $x_0, x_1, \dots, x_n$ and coefficients $A_0, A_1, \dots, A_n$ (which are also called weights) to minimize the expected error obtained in the approximation:

$$\int_a^b f(x)\ dx \approx \sum_{i=0}^{n} A_i f(x_i)$$

To measure this accuracy, we assume that the best choice of theses values is that which produces the exact result for the largest class of polynomials.

Derive for the case $n = 1$

$n = 1$, then we have:

$$\int_{-1}^{1} f(x)\ dx = A_0 f(x_0) + A_1 \cdot f(x_1)$$

Suppose that $f(x) = x^j \quad j = 0, 1, 2, 3$

$$\int_{-1}^{1} x^j\ dx = \frac{1}{j+1} x^{j+1} \bigg|_{-1}^{1}$$

Then we can have the four equations:

$$\begin{aligned} 2 &= A_0 + A_1 && (1) \\ 0 &= A_0 \cdot x_0 + A_1 \cdot x_1 && (2) \\ \frac{2}{3} &= A_0 \cdot x_0^2 + A_1 \cdot x_1^2 && (3) \\ 0 &= A_0 \cdot x_0^3 + A_1 \cdot x_1^3 && (4) \end{aligned}$$

From Equation(2), we know that $A_0 \cdot x_0 = -A_1 \cdot x_1$, we use this into Equation(4), which gives us:

$$A_1 \cdot x_1^3 - A_1 \cdot x_1 \cdot x_0^2 = 0 \implies A_1 \cdot x_1 \cdot (x_1^2 - x_0^2) = 0$$

It is impossible for $A_1 \cdot x_1 = 0$, otherwise according to Equation(2), $A_0 \cdot x_0 = 0$ contradicts with Equation(3).

Thus we have $x_1^2 = x_0^2$. It is also impossible for $x_1 = x_0$(We have shown $A_1 \cdot x_1 \neq 0$). Otherwise, we will imply that $A_0 + A_1 = 0$ from Equation(2), which contradicts with Equation(1).

Then, we can say that $x_1 = -x_2 \implies A_0 = A_1 = 1 \implies x_0 = \frac{1}{\sqrt{3}}, x_1 = -\frac{1}{\sqrt{3}}$

Thus, we have:

$$\int_{-1}^{1} f(x)\ dx = 1 \cdot f(\frac{1}{\sqrt{3}}) + 1 \cdot f(-\frac{1}{\sqrt{3}})$$

Question:
What is the highest degree of polynomials for

$$\int_a^b f(x)\ dx = \sum_{i=0}^{n} A_i \cdot f(x_i) \tag{4}$$

holds by choosing $x_i, i = 0, 1, 2, \ldots, n$

Take $f(x) = x^j, \quad j = 0, 1, \ldots, m$

$$\int_a^b x^j\ dx = \sum_{i=0}^{n} A_i \cdot x_i^j \qquad j = 0, 1, \ldots, m$$

From above, we know there are $m+1$ equations.
From Equation(4), we know that there are $A_0, x_0, A_1, x_1, \ldots, A_n, x_n$, total $2n+2$ unknowns.

Thus, we have $m+1 \leq 2n+2 \implies m \leq 2n+1$

For any polynomial $f(x)$ of degree $\leq 2n+1$.
We can do linear combinations:

$$f(x) = c_0 + c_1 \cdot x + \ldots + c_{2n+1} \cdot x^{2n+1}$$

$$\begin{aligned}
\int_a^b f(x)\ dx &= \sum_{j=0}^{2n+1} c_j \int_a^b x^j\ dx \\
&= \sum_{j=0}^{2n+1} c_j \sum_{i=0}^{n} A_i \cdot x_i^i \\
&= \sum_{i=0}^{n} A_i \sum_{j=0}^{2n+1} c_j \cdot x_i^i \\
&= \sum_{i=0}^{n} A_i f(x_i)
\end{aligned}$$

NOTE: If the number of equations is larger than the number of unknowns, you may not have a solution, e,g., two equations and one unknown: $x = 1, x = 2$. If you have one equation with two unknowns, e.g., $x + y = 2$, you have many solutions.

What we want here is to make sure there are solution, we don't have to have unique solution, right?

Interval change:

Suppose a Gaussian quadrature rule for $\int_{-1}^{1} f(x)\ dx$ is

$$I_G[-1,1] = \sum_{i=0}^{n} A_i \cdot f(x_i)$$

We can extend it to compute $\int_a^b f(x)\ dx$ by an interval transformation.

Suppose that $x \in [a,b] \implies x = \alpha + \beta \cdot t \in [a,b]$, in which $t \in [-1,1]$, then we have:

$$\begin{cases} \alpha + \beta = b \\ \alpha - \beta = a \end{cases} \implies \begin{cases} \alpha = \dfrac{1}{2} \cdot (a+b) \\ \\ \beta = \dfrac{1}{2} \cdot (b-a) \end{cases}$$

Then we have:

$$\int_a^b f(x)\ dx = \beta \int_{-1}^{1} f(\alpha + \beta t)\ dt \approx I_G[a,b] \equiv \beta \cdot \sum_{i=0}^{n} A_i \cdot f(\alpha + \beta \cdot x_i)$$

An Example

Suppose we want to compute $\int_a^b f(x)\ dx$. We divide the interval $[a,b]$ into n equal subintervals $[x_i, x_{i+1}]$, $i = 0, 1, \ldots, n-1$. For each subinterval we apply the Gaussian two-point quadrature rule, leading to the composite Gaussian two-point quadrature rule.

Let $x = \dfrac{b-a}{2} t + \dfrac{a+b}{2}$

$$\begin{aligned} \int_a^b f(x)\ dx &= \frac{b-a}{2} \int_{-1}^{1} f(\frac{b-a}{2} t + \frac{a+b}{2})\ dt \\ &\approx \frac{b-a}{2} \left[f\Big(\frac{b-a}{2} \cdot (-\frac{\sqrt{3}}{3}) + \frac{a+b}{2} \Big) + f\Big(\frac{b-a}{2} \cdot \frac{\sqrt{3}}{3} + \frac{a+b}{2} \Big) \right] \end{aligned}$$

Then divide $[a,b]$ into n intervals, and apply the formula above, we have:

$$\begin{aligned} \int_a^b f(x)\ dx &= \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} f(x)\ dx \qquad (x_i = a + i \cdot h, h = \frac{b-a}{n}) \\ &\approx \frac{h}{2} \cdot \sum_{i=0}^{n-1} \left[f\Big(-\frac{h}{2\sqrt{3}} + \frac{a + ih + a + (i+1) \cdot h}{2} \Big) \right] + \left[f\Big(\frac{h}{2\sqrt{3}} + \frac{a + ih + a + (i+1) \cdot h}{2} \Big) \right] \\ &= \frac{h}{2} \cdot \sum_{i=0}^{n-1} \left[f\Big(-\frac{h}{2\sqrt{3}} + a + ih + \frac{h}{2} \Big) \right] + \left[f\Big(\frac{h}{2\sqrt{3}} + a + ih + \frac{h}{2} \Big) \right] \end{aligned}$$