Homework 1

Math 651
Fall 2019

Due Friday, September 20

The following was left as an exercise in our development of adaptive quadrature.

Problem 1 (3 points)**.** Let $f \in C^4$. Show using Taylor's theorem that for any x,

$$\frac{f''(x-h)+f''(x+h)}{2} = f''(x) + O(h^2)$$

in the limit as $h \to 0$.

In general, quadratures take the form

$$\int_0^1 f\,dx \approx Q_{[0,1]}f := \sum_{i=1}^{K} w_i f(x_i), \tag{1}$$

for some *weights* $w_i \in \mathbb{R}$ and *nodes* $x_i \in [0,1]$. Given such a quadrature $Q_{[0,1]}$ for the interval $[0,1]$, we define a corresponding quadrature $Q_{[a,b]}$ for the arbitrary interval $[a,b]$ by making the change of variable

$$u = (b-a)x + a.$$

This yields

$$\begin{aligned}
\int_a^b f\,dx &= (b-a)\int_0^1 f \circ u\,dx \\
&\approx (b-a)\sum_{i=1}^{K} w_i f \circ u(x_i) \\
&= (b-a)\sum_{i=1}^{K} w_i f(x_i b + (1-x_i)a) \\
&=: Q_{[a,b]}f.
\end{aligned}$$

We also define a composite quadrature by

$$Q_{[a,b]}^N f = \sum_{i=1}^{N} Q_{[a+(i-1)h,a+ih]}f,$$

where

$$h = \frac{b-a}{N}.$$

Quadratures are often compared based on their *degree of precision*: A quadrature is said to have degree of precision k if it is exact for polynomials of degree less than or equal to k; that is, if

$$\int_0^1 p\,dx = Q_{[0,1]}p$$

for all polynomials $p \in \cup_{m \le k} \mathscr{P}^m$. Quadratures with higher degree of precision usually (but not always) perform better than quadratures with lower degree of precision. The following problem explains why a high degree of precision might be a good thing.

Problem 2 (4+3+2 points)**.** Let $Q_{[0,1]}$ be a quadrature of form (1) with degree of precision k. Define the error

$$E_{[a,b]}f := \int_a^b f\,dx - Q_{[a,b]}f.$$

1. Let $f \in C^{k+1}([0,1])$. Use Taylor's Theorem to show that

   $$\left|E_{[0,1]}f\right| \le C \left\|f^{(k+1)}\right\|_{L^\infty([0,1])} \tag{2}$$

   for some constant C depending on k and the weights w_i but not on f.

   Hint: The quadrature $Q_{[0,1]}$ integrates the polynomial part of a $k+1$ term Taylor expansion exactly.

2. Let $g \in C^{k+1}([a,b])$. Show by the change of variable $u = (b-a)x + a$ that

   $$\left|E_{[a,b]}g\right| \le C(b-a)^{k+2} \left\|g^{(k+1)}\right\|_{L^\infty([a,b])}.$$

3. Show that

   $$\begin{aligned}\left|E^N_{[a,b]}f\right| &:= \left|\int_a^b f\,dx - Q^N_{[a,b]}f\right| \\ &\le C(b-a)h^{k+1}\left\|f^{(k+1)}\right\|_{L^\infty([a,b])} \\ &= \frac{C(b-a)^{k+2}\left\|f^{(k+1)}\right\|_{L^\infty([a,b])}}{N^{k+1}}.\end{aligned}$$

We have just seen the use of Lagrange interpolation to derive quadratures with a high degree of precision. However, there are other ways to derive such high order methods. For example, the following problem develops a special case of a general technique called *Richardson extrapolation.*

Problem 3 (3+2 points)**.** In this problem, we use the notation introduced in class for the composite midpoint rule. We let $a = x_0 < x_1 < \cdots < x_N = b$ be a partition of $[a, b]$, and we define $J_i = [x_{i-1}, x_i]$ and $h_i = x_i - x_{i-1}$ for $i = 1, \ldots, N$.

1. Recall that if $f \in C^4$, then

$$\int_{J_i} f(x)\,dx - M_{J_i} f = C h_i^3 + O(h_i^5), \text{ and}$$
$$\int_{J_i} f(x)\,dx - M_{J_i}^2 f = \frac{C}{4} h_i^3 + O(h_i^5),$$

   where

$$C = \frac{f''\left(\frac{x_i + x_{i-1}}{2}\right)}{24}.$$

   Let

$$\tilde{M}_{J_i} f := M_{J_i} f + \frac{4}{3}(M_{J_i}^2 f - M_{J_i} f).$$

   Show that

$$\int_{J_i} f(x)\,dx - \tilde{M}_{J_i} f = O(h_i^5).$$

   That is, $\tilde{M}_{J_i}$ is fifth order accurate as h_i tends to zero, whereas M_{J_i} is only third order accurate.

2. What are the weights and nodes corresponding to $\tilde{M}_{[0,1]}$?

Problem 4 (2+2+5+1+1 points)**.** Simpson's rule is the quadrature

$$S_{[0,1]} f = \frac{1}{6} f(0) + \frac{2}{3} f(1/2) + \frac{1}{6} f(1).$$

1. What is the maximal degree of precision of Simpson's rule? *Hint:* Simply check whether Simpson's rule exactly integrates x^k for each $k = 0, 1, 2, \ldots$ in sequence. As you increase k, you will find a monomial x^j for which Simpson's rule is not exact. The maximal degree of precision will be $j - 1$.

2. Show that Simpson's rule is the Newton–Cotes quadrature with $n = 3$. Given this fact, do you find the maximal degree of precision of Simpson's rule surprising?

3. Perform a convergence study for the composite version of Simpson's rule.

To be precise, define

$$
\begin{aligned}
f(x) &= \exp(x), \\
g(x) &= \sqrt{x}, \text{ and} \\
q(x) &= \begin{cases} 0 & \text{if } x \le \pi \\ x - \pi & \text{if } x \ge \pi. \end{cases} \\
r(x) &= \begin{cases} 0 & \text{if } x \le \pi \\ (x - \pi)^2 & \text{if } x \ge \pi. \end{cases}
\end{aligned}
$$

Compute $S_{[0,4]}^N z$ for $z \in \{f, g, q, r\}$ and $N \in \{2^k; k = 0, \ldots, 12\}$. Define the error

$$E_{[0,4]}^N z = \int_0^4 z(x)\,dx - S_{[0,4]}^N z.$$

For each $z \in \{f, g, q, r\}$, plot $\log_{10}(E_{[0,4]}^N z)$ versus $\log_{10}(N)$. Are the curves in the plots roughly linear, and if so what are their slopes? Do your observations agree with the theory developed in Problem 2?

Hint: If you like, you can imitate the example given at `http://people.math.umass.edu/~vankoten/2019-fall-math651/notebooks/python-examples.html`. This problem will be easy if you make a function that does the entire convergence study, including the plots, for a given integrand.

4. You will have seen that Simpson's rule does not converge at the predicted rate for $q(x)$ and also some of the other functions. Suppose you know that a function $w(x)$ is analytic on $[0, \pi)$ and $(\pi, 4]$ but has a jump in its derivative at π. How would you implement the composite Simpson's rule for $w(x)$ to get the rate of convergence predicted by the theory developed in Problem 2?

5. How might you decide which of Simpson's rule and $\tilde{M}$ is better? What information do you need to have to make the decision? *Hint:* Think about implementations. It turns out that S and $\tilde{M}$ have have the same degree of precision. (You don't have to prove this.) Do their composite forms require the same number of function evaluations for a given N?

As we have seen, asymptotic expansions of the error yield practical error estimates and efficient adaptive quadrature methods. However, since the error estimates rely on asymptotics, one can only guarantee their validity in the limit of small h_i. Thus, while asymptotic estimates often work beautifully, one must be skeptical. In Problem 5, I ask that you find an integrand f for which our midpoint rule error estimate fails.

Problem 5 (3 points)**.** Find a function $f \in C^4([0,1])$ so that

$$M_{[0,1]}f - M^2_{[0,1]}f = 0,$$

but

$$\left| \int_0^1 f\,dx - M_{[0,1]}f \right| \geq 1.$$

Note: You may simply draw the graph of such a function, provided that you label the relevant features of the graph and offer a convincing explanation.