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Lecture 30 Notes

These notes correspond to Section 4.6 in the text.

Adaptive Quadrature

Composite rules can be used to implement an *automatic* quadrature procedure, in which the all of the subintervals of $[a, b]$ are continually subdivided until sufficient accuracy is achieved. However, this approach is impractical since small subintervals are not necessary in regions where the integrand is smooth.

An alternative is *adaptive quadrature*. Adaptive quadrature is a technique in which the interval $[a, b]$ is divided into n subintervals $[a_j, b_j]$, for $j = 0, 1, \dots, n - 1$, and a quadrature rule, such as the Trapezoidal Rule, is used on each subinterval to compute

$$I_j(f) = \int_{a_j}^{b_j} f(x) dx,$$

as in any composite quadrature rule. However, in adaptive quadrature, a subinterval $[a_j, b_j]$ is subdivided if it is determined that the quadrature rule has not computed $I_j(f)$ with sufficient accuracy.

To make this determination, we use the quadrature rule on $[a_j, b_j]$ to obtain an approximation I_1 , and then use the corresponding composite rule on $[a_j, b_j]$, with two subintervals, to compute a second approximation I_2 . If I_1 and I_2 are sufficiently close, then it is reasonable to conclude that these two approximations are accurate, so there is no need to subdivide $[a_j, b_j]$. Otherwise, we divide $[a_j, b_j]$ into two subintervals, and repeat this process on these subintervals. We apply this technique to all subintervals, until we can determine that the integral of f over each one has been computed with sufficient accuracy. By subdividing only when it is necessary, we avoid unnecessary computation and obtain the same accuracy as with composite rules or automatic quadrature procedures, but with much less computational effort.

We now describe an algorithm for adaptive quadrature. This algorithm uses the Trapezoidal Rule to integrate over intervals, and intervals are subdivided as necessary into two subintervals of equal width. The algorithm uses a data structure called a *stack* in order to keep track of the subintervals over which f still needs to be integrated. A stack is essentially a list of elements, where the elements, in this case, are subintervals. An element is added to the stack using a *push* operation, and is removed using a *pop* operation. A stack is often described using the phrase “last-in-first-out,” because the most recent element to be pushed onto the stack is the first element to be popped. This corresponds to our intuitive notion of a stack of objects, in which objects are placed on top of the stack and are removed from the top as well.

Algorithm (Adaptive Quadrature) Given a function $f(x)$ that is integrable on an interval $[a, b]$, the following algorithm computes an approximation I to $I(f) = \int_a^b f(x) dx$ that is accurate to within $(b - a)TOL$, where TOL is a given error tolerance.

S is an empty stack

$push(S, [a, b])$

$I = 0$

while S is not empty **do**

$[a, b] = pop(S)$ (the interval $[a, b]$ on top of S is removed from S)

$I_1 = [(b - a)/2][f(a) + f(b)]$ (Trapezoidal Rule)

$m = (a + b)/2$

$I_2 = [(b - a)/4][f(a) + 2f(m) + f(b)]$ (Composite Trapezoidal Rule with 2 subintervals)

if $|I_1 - I_2| < 3(b - a)TOL$ **then**

$I = I + I_2$ (from error term in Trapezoidal Rule, $|I(f) - I_2| \approx \frac{1}{3}|I_1 - I_2|$)

else

$push(S, [a, m])$

$push(S, [m, b])$

end

end

Throughout the execution of the loop in the above algorithm, the stack S contains all intervals over which f still needs to be integrated to within the desired accuracy. Initially, the only such interval is the original interval $[a, b]$. As long as intervals remain in the stack, the interval on top of the stack is removed, and we attempt to integrate over it. If we obtain a sufficiently accurate result, then we are finished with the interval. Otherwise, the interval is bisected into two subintervals, both of which are pushed on the stack so that they can be processed later. Once the stack is empty, we know that we have accurately integrated f over a collection of intervals whose union is the original interval $[a, b]$, so the algorithm can terminate.

Example We will use *adaptive quadrature* to compute the integral

$$\int_0^{\pi/4} e^{3x} \sin 2x dx$$

to within $(\pi/4)10^{-4}$.

Let $f(x) = e^{3x} \sin 2x$ denote the integrand. First, we use Simpson's Rule, or, equivalently, the Composite Simpson's Rule with $n = 2$ subintervals, to obtain an approximation I_1 to this integral. We have

$$I_1 = \frac{\pi/4}{6}[f(0) + 4f(\pi/8) + f(\pi/4)] = 2.58369640324748.$$

Then, we divide the interval $[0, \pi/4]$ into two subintervals of equal width, $[0, \pi/8]$ and $[\pi/8, \pi/4]$, and integrate over each one using Simpson's Rule to obtain a second approximation I_2 . This is

equivalent to using the Composite Simpson's Rule on $[0, \pi/4]$ with $n = 4$ subintervals. We obtain

$$\begin{aligned} I_2 &= \frac{\pi/8}{6}[f(0) + 4f(\pi/16) + f(\pi/8)] + \frac{\pi/8}{6}[f(\pi/8) + 4f(3\pi/16) + f(\pi/4)] \\ &= \frac{\pi/16}{3}[f(0) + 4f(\pi/16) + 2f(\pi/8) + 4f(3\pi/16) + f(\pi/4)] \\ &= 2.58770145345862. \end{aligned}$$

Now, we need to determine whether the approximation I_2 is sufficiently accurate. Because the error in the Composite Simpson's Rule is $O(h^4)$, where h is the width of each subinterval used in the rule, it follows that the actual error in I_2 satisfies

$$|I_2 - I(f)| \approx \frac{1}{15}|I_2 - I_1|,$$

where $I_f(f)$ is the exact value of the integral of f .

We find that the relation

$$|I_2 - I(f)| \approx \frac{1}{15}|I_2 - I_1| < \frac{\pi}{4}10^{-4}$$

is *not* satisfied, so we must divide the interval $[0, \pi/4]$ into two subintervals of equal width, $[0, \pi/8]$ and $[\pi/8, \pi/4]$, and use the Composite Simpson's Rule with these smaller intervals in order to achieve the desired accuracy.

First, we work with the interval $[0, \pi/8]$. Proceeding as before, we use the Composite Simpson's Rule with $n = 2$ and $n = 4$ subintervals to obtain approximations I_1 and I_2 to the integral of $f(x)$ over this interval. We have

$$I_1 = \frac{\pi/8}{6}[f(0) + 4f(\pi/16) + f(\pi/8)] = 0.33088926959519.$$

and

$$\begin{aligned} I_2 &= \frac{\pi/16}{6}[f(0) + 4f(\pi/32) + f(\pi/16)] + \frac{\pi/16}{6}[f(\pi/16) + 4f(3\pi/32) + f(\pi/8)] \\ &= \frac{\pi/32}{3}[f(0) + 4f(\pi/32) + 2f(\pi/16) + 4f(3\pi/32) + f(\pi/8)] \\ &= 0.33054510467064. \end{aligned}$$

Since these approximations satisfy the relation

$$|I_2 - I(f)| \approx \frac{1}{15}|I_2 - I_1| < \frac{\pi}{8}10^{-4},$$

where $I(f)$ denotes the exact value of the integral of f over $[0, \pi/8]$, we have achieved sufficient accuracy on this interval and we do not need to subdivide it further. The more accurate approximation I_2 can be included in our approximation to the integral over the original interval $[0, \pi/4]$.

Now, we need to achieve sufficient accuracy on the remaining subinterval, $[\pi/4, \pi/8]$. As before, we compute the approximations I_1 and I_2 of the integral of f over this interval and obtain

$$I_1 = \frac{\pi/8}{6}[f(\pi/8) + 4f(3\pi/16) + f(\pi/4)] = 2.25681218386343.$$

and

$$\begin{aligned} I_2 &= \frac{\pi/16}{6}[f(\pi/8) + 4f(5\pi/32) + f(3\pi/16)] + \frac{\pi/16}{6}[f(3\pi/16) + 4f(7\pi/32) + f(\pi/4)] \\ &= \frac{\pi/32}{3}[f(\pi/8) + 4f(5\pi/32) + 2f(3\pi/16) + 4f(7\pi/32) + f(\pi/4)] \\ &= 2.25801455892266. \end{aligned}$$

Since these approximations do not satisfy the relation

$$|I_2 - I(f)| \approx \frac{1}{15}|I_2 - I_1| < \frac{\pi}{8}10^{-4},$$

where $I(f)$ denotes the exact value of the integral of f over $[\pi/8, \pi/4]$, we have not achieved sufficient accuracy on this interval and we need to subdivide it into two subintervals of equal width, $[\pi/8, 3\pi/16]$ and $[3\pi/16, \pi/4]$, and use the Composite Simpson's Rule with these smaller intervals in order to achieve the desired accuracy.

The discrepancy in these two approximations to the integral of f over $[\pi/4, \pi/8]$ is larger than the discrepancy in the two approximations of the integral over $[0, \pi/8]$ because even though these intervals have the same width, the derivatives of f are larger on $[\pi/8, \pi/4]$, and therefore the error in the Composite Simpson's Rule is larger.

We continue the process of adaptive quadrature on the interval $[\pi/8, 3\pi/16]$. As before, we compute the approximations I_1 and I_2 of the integral of f over this interval and obtain

$$I_1 = \frac{\pi/16}{6}[f(\pi/8) + 4f(5\pi/32) + f(3\pi/16)] = 0.72676545197054.$$

and

$$\begin{aligned} I_2 &= \frac{\pi/32}{6}[f(\pi/8) + 4f(9\pi/64) + f(5\pi/32)] + \frac{\pi/32}{6}[f(5\pi/32) + 4f(11\pi/64) + f(3\pi/16)] \\ &= \frac{\pi/64}{3}[f(\pi/8) + 4f(9\pi/64) + 2f(5\pi/32) + 4f(11\pi/64) + f(3\pi/16)] \\ &= 0.72677918153379. \end{aligned}$$

Since these approximations satisfy the relation

$$|I_2 - I(f)| \approx \frac{1}{15}|I_2 - I_1| < \frac{\pi}{16}10^{-4},$$

where $I(f)$ denotes the exact value of the integral of f over $[\pi/8, 3\pi/16]$, we have achieved sufficient accuracy on this interval and we do not need to subdivide it further. The more accurate approximation I_2 can be included in our approximation to the integral over the original interval $[0, \pi/4]$.

Now, we work with the interval $[3\pi/16, \pi/4]$. Proceeding as before, we use the Composite Simpson's Rule with $n = 2$ and $n = 4$ subintervals to obtain approximations I_1 and I_2 to the integral of $f(x)$ over this interval. We have

$$I_1 = \frac{\pi/16}{6}[f(3\pi/16) + 4f(7\pi/32) + f(\pi/4)] = 1.53124910695212.$$

and

$$\begin{aligned} I_2 &= \frac{\pi/32}{6}[f(3\pi/16) + 4f(13\pi/64) + f(7\pi/32)] + \frac{\pi/32}{6}[f(7\pi/32) + 4f(15\pi/64) + f(\pi/4)] \\ &= \frac{\pi/64}{3}[f(3\pi/16) + 4f(13\pi/64) + 2f(7\pi/32) + 4f(15\pi/64) + f(\pi/4)] \\ &= 1.53131941583939. \end{aligned}$$

Since these approximations satisfy the relation

$$|I_2 - I(f)| \approx \frac{1}{15}|I_2 - I_1| < \frac{\pi}{16}10^{-4},$$

where $I(f)$ denotes the exact value of the integral of f over $[3\pi/16, \pi/4]$, we have achieved sufficient accuracy on this interval and we do not need to subdivide it further. The more accurate approximation I_2 can be included in our approximation to the integral over the original interval $[0, \pi/4]$.

We conclude that the integral of $f(x)$ over $[0, \pi/4]$ can be approximated by the sum of our approximate integrals over $[0, \pi/8]$, $[\pi/8, 3\pi/16]$, and $[3\pi/16, \pi/4]$, which yields

$$\begin{aligned} \int_0^{\pi/4} e^{3x} \sin 2x \, dx &\approx 0.33054510467064 + 0.72677918153379 + 1.53131941583939 \\ &\approx 2.58864370204382. \end{aligned}$$

Since the exact value is 2.58862863250716, the absolute error is -1.507×10^{-5} , which is less in magnitude than our desired error bound of $(\pi/4)10^{-4} \approx 7.854 \times 10^{-5}$. This is because on each subinterval, we ensured that our approximation was accurate to within 10^{-4} times the width of the subinterval, so that when we added these approximations, the total error in the sum would be bounded by 10^{-4} times the width of the union of these subintervals, which is the original interval $[0, \pi/4]$. \square

Adaptive quadrature can be very effective, but it should be used cautiously, for the following reasons:

- The integrand is only evaluated at a few points within each subinterval. Such sampling can miss a portion of the integrand whose contribution to the integral can be misjudged.
- Regions in which the function is not smooth will still only make a small contribution to the integral if the region itself is small, so this should be taken into account to avoid unnecessary function evaluations.
- Adaptive quadrature can be very inefficient if the integrand has a discontinuity within a subinterval, since repeated subdivision will occur. This is unnecessary if the integrand is smooth on either side of the discontinuity, so subintervals should be chosen so that discontinuities occur between subintervals whenever possible.