Adaptive Quadrature

Math 131: Numerical Analysis

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Section 1

Introduction

Adaptive Quadrature

- Composite quadrature formulas can be quite effective as we discussed in the last section.
- There is one drawback however - so far we have only used a uniform spacing for the nodes.
- We did this mainly to simplify the analysis, and to highlight the main ideas. However, there was no underlying need to do so.
- In fact, there are many situations where it is clear that a uniform spacing might not be optimal.

Example

Consider for example:

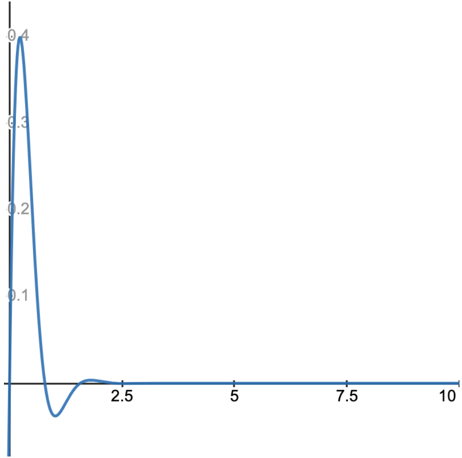

Figure 1: $f(x) = e^{-3x}\sin(4x),\ x \in [0, 10]$

Uniform spacing

- If we attempt to use a **uniform spacing** that tries to approximate the integral of this function, we will be caught between two competing interests.
- To capture the behavior of the function towards the right end of the interval a spacing of $h = 0.5$ or even $h = 1.0$ would likely be adequate.
- However, if we want to capture the behavior of the function towards the left end of the interval, then it looks likely that we would need to have a spacing of h that is much smaller.
- And if we choose the smaller h then we will be committed to doing additional computational work that is not needed on the right end of the interval.

Uniform spacing in higher dimensinos

- This problem can be exacerbated when working in two or three dimensions, where the computational work could increase dramatically, if we have to choose a uniform h in all of the dimensions.
- In the above example, suppose we had to choose one h for the entire region. The table below depicts the size of the problem in terms of the number of "cells" one would have to compute over the interval $[0, 10]$ with a uniform grid, and a nonuniform grid where the majority of the points are chosen in a small subinterval, say $x \in [0, 2]$.
- The difference isn't particularly noteworthy in one dimension but when you reach a three-dimensional problem, there is an additional factor of 1000 to consider when using a uniform grid.

Uniform spacing in higher dimensions

Type	h	N	N^2	N^3
Uniform	0.1	100	$\approx 10^4$	$\approx 10^6$
	0.01	1000	$\approx 10^6$	$\approx 10^9$
Nonuniform	0.1	≈ 20	≈ 400	≈ 8000
	0.01	≈ 110	$\approx 10^4$	$\approx 10^6$

Grid on $[0, 10]$

Idea

- The solution is obvious, which is to find a value of h that is adapted to what the function is doing over a particular subinterval.
- But the big question is how do we know this without evaluating the function at many different points and
- How do we choose a good value of h that gives us good accuracy without also increasing the computational workload too much.

Idea

If we could predict the variation in the function, then we could choose a smaller h in only those regions that need it to attain the accuracy we want! Our strategy will be to leverage our **error analysis** to help us predict the variation.

Section 2

Romberg Integration

Composite Trapezoid Error Analysis

Let's consider the Composite Trapezoid Rule first. Recall that we can write the quadrature formula as:

$$I(f) = \int_a^b f(x)dx = \frac{h}{2}\left[f(a) + 2\sum_{i=1}^{r-1} f(t_i) + f(b)\right] - \frac{(b-a)}{12}h^2 f''(\mu),$$

As before with Richardson extrapolation, let's break this approximation down into 2 parts. This approach is also called ***Romberg integration.***

(cont.)

Suppose we write the approximation to the integral as:

$$R_1 = \frac{h}{2}\Big[f(a) + 2f(a+h) + ... + 2f(b-h) + f(b)\Big] + Kh^2,$$

Now let's suppose we cut h in half and write the Composite Trapezoid rule again:

$$R_2 = \frac{h}{4}\Big[f(a) + 2f(a+h/2) + ... + 2f(b-h/2) + f(b)\Big] + K\Big(\frac{h}{2}\Big)^2,$$

(cont.)

Let's now consider the error in each of these formulas:

$$
\begin{aligned}
I(f) - R_1 &\approx Kh^2, \\
I(f) - R_2 &\approx K\left(\frac{h}{2}\right)^2 = \frac{1}{4}Kh^2.
\end{aligned}
$$

Caution

The next step requires us to make an assumption, namely that the terms that constitute the constant K in both of the above terms are approximately equal.

This should be true if the fourth derivative terms in each of the constants are comparable, which seems reasonable since they are from the same function and over similar intervals:

$$f^{(4)}(\mu_1) \approx f^{(4)}(\mu_2).$$

(cont.)

Substituting the first equation into the second we get:

$$I(f) - R_2 \approx \frac{1}{4}[I(f) - R_1]. \tag{1}$$

Let's now consider the error for R_1:

$$\begin{aligned} I(f) - R_1 &= (I(f) - R_2) + (R_2 - R_1), \\ &\approx \frac{1}{4}[I(f) - R_1] + (R_2 - R_1) \end{aligned} \tag{2}$$

$$\implies I(f) - R_1 \approx \frac{4}{3}(R_2 - R_1).$$

a posteriori error estimates

Finally, we can combine Equation 1 and Equation 2 to get:

$$\begin{aligned} I(f) - R_2 &\approx \frac{1}{4}[I(f) - R_1] \\ &\approx \frac{1}{4}\Big[\frac{4}{3}(R_2 - R_1)\Big] \end{aligned} \tag{3}$$

$$\implies I(f) - R_2 \approx \frac{1}{3}\Big[(R_2 - R_1)\Big]$$

The important thing to note is that once everything on the right hand sides (specifically R_1, R_2), have been computed, we can generate an estimate for the error in both quadrature approximations. These types of computations are known as ***a posteriori error*** estimates.

Summarizing Composite Trapezoid *a posteriori* estimates

Composite Trapezoid *a posteriori* error estimates

$$I(f) - R_1 \approx \frac{4}{3}\Big(R_2 - R_1\Big),$$
$$I(f) - R_2 \approx \frac{1}{3}\Big(R_2 - R_1\Big).$$

We can interpret this to mean that the error from the quadrature approximation for R_2 (with $h/2$) should be about $1/3$ of the difference between the two Trapezoid rule approximations at h and $h/2$.

Composite Simpson's *a posteriori* estimates

In a similar manner we can produce *a posteriori* error estimates for composite Simpson's rule and write:

Simpson *a posteriori* error estimates

$$
\begin{aligned}
I(f) - S_1 &\approx \frac{16}{15}\Big(S_2 - S_1\Big), \\
I(f) - S_2 &\approx \frac{1}{15}\Big(S_2 - S_1\Big).
\end{aligned}
$$

We can interpret this to mean that the error from the quadrature approximation with $h/2$ (S_2) should be about $1/15$ of the difference between the two Simpson's rule approximations at h and $h/2$.

Strategy for adaptively choosing h

- These observations can lead us to develop a strategy for deciding when to subdivide a panel and when to stop.
- Specifically, suppose we want the error to be less than a certain tolerance, ϵ, for Composite Simpson's Rule.
- Then we can ask whether for a given panel

$$\frac{1}{15}\left(S_2 - S_1\right) < \epsilon.$$

If this is true, then we can stop for that given panel. If however, the difference doesn't satisfy the tolerance, that is an indication that we should subdivide the region in half again.

General Algorithm

A general algorithm might look something like:

1. Initialize by computing Simpson's on $[a, b]$, i.e. S_1
2. For $i = 1, 2, ...$
    1. subdivide the interval into 2 sub-regions and compute S_{i+1} by applying Simpson on each subinterval
    2. If $|S_{i+1} - S_i| < 15\epsilon$
        1. converged
        2. else repeat.

Section 3

Summary

Summary

- This is just a brief introduction into adaptive quadrature.
- The main point to remember is that using our error analysis can help us choose better values of h so that we get better approximations to our integrals.
- There are many other techniques one can use to improve both the accuracy and the efficiency of these methods.
- An interested reader, can find many references under topics such as adaptive mesh refinement.