Composite Quadrature Rules

Math 131: Numerical Analysis

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Section 1

Composite Integration

Composite Integration

In practice we can't use Newton-Cotes over large intervals as it would require high degree polynomials, which would be unsuitable due to the highly oscillatory nature. Another disadvantage is that we would need to have equally spaced intervals, which are not suitable for many physical applications.

Idea

Instead of trying to approximate the integral accurately over the entire interval with one polynomial, break up the domain into smaller regions and use low-order polynomials on each of them.

Multiple Panels

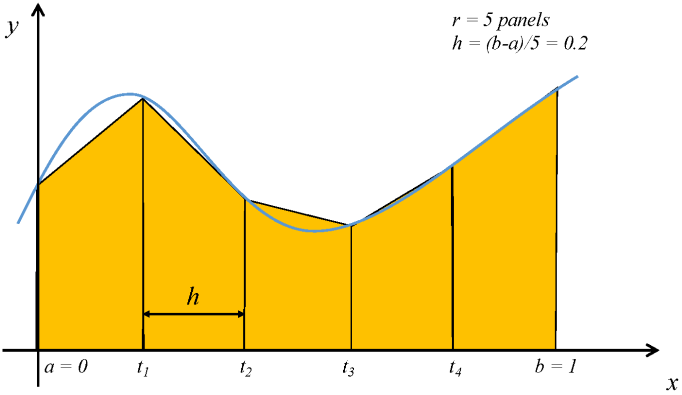

Figure 1: Approximating the integral by sudviding the region into multiple "panels" and using the trapezoid rule will lead to higher accuracy

Strategy

- The strategy is to use something simple like Trapezoid or Simpson's Rule on each of the subregions (often called ***panels***), and then sum up the individual contributions to arrive at the solution to the original problem.
- There is nothing in this approach that directs us to use subregions of equal size, but for exposition, we will assume that they are for the time being. We will come back to this point in the next section on adaptive methods.
- In the general case, let's assume that we have sub-divided the interval $[a, b]$ Into r subregions, each of equal length $h = \frac{b-a}{r}$. See Figure 1 for the case $r = 5$.

(cont.)

Our composite quadrature rule could then be written as:

$$\int_a^b f(x)dx = \sum_{i=1}^{r} \int_{t_{i-1}}^{t_i} f(x)dx,$$

where $t_i = a + ih$.

All we need do now is to apply one of our earlier quadrature formulas to the integrals in each of the subintervals $[t_{i-1}, t_i]$.

Example

Let's work out an example in the simple case of the Trapezoid Rule:

$$
\begin{aligned}
\int_a^b f(x)dx &\approx \sum_{i=1}^{r} \int_{t_{i-1}}^{t_i} f(x)dx, \\
&\approx \sum_{i=1}^{r} \frac{h}{2}\left[f(t_{i-1}) + f(t_i)\right], \\
&= \frac{h}{2}\left[f(t_0) + 2f(t_1) + 2f(t_2) + \ldots + 2f(t_{r-1}) + f(t_r)\right], \\
&= \frac{h}{2}\left[f(a) + 2f(t_1) + 2f(t_2) + \ldots + 2f(t_{r-1}) + f(b)\right],
\end{aligned}
$$

Composite Trapezoidal Rule

This leads to the Composite Trapezoid Rule:

Composite Trapezoidal Rule

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

where $h = (b-a)/r$; $t_i = a + ih,\ i = 0, 1, \ldots, r$ and $\mu \in (a, b)$.

Composite Simpson's

A similar exercise will lead to the Composite Simpson's Rule:

Composite Simpson's Rule

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}[f(a) + 2\sum_{i=1}^{r/2-1} f(t_{2i}) + 4\sum_{i=1}^{r/2} f(t_{2i-1}) + f(b)] \\ - \frac{(b-a)}{180}h^4 f^{(4)}(\mu). \tag{2}$$

where $h = (b-a)/r$; $t_i = a + ih,\ i = 0, 1, \ldots, r$ and $\mu \in (a, b)$.

(cont.)

- The derivation for Composite Simpson's rule isn't difficult, and mostly a matter of getting the right indices.
- One observation that is helpful in deriving the formula is that because of the need for 3 nodes in Simpson's rule we should consider the panels in pairs.
- For this reason, ***the number of panels for Simpson's rule must always be an even number.***

Example

Let's consider the simplest case with 4 panels, which we can group into two pairs, as depicted in the figure below. Here you should think of the first integration region spanning the first two panels so as to encompass the area in the interval $[t_0, t_2]$. Likewise, the second region will cover the interval $[t_2, t_4]$.

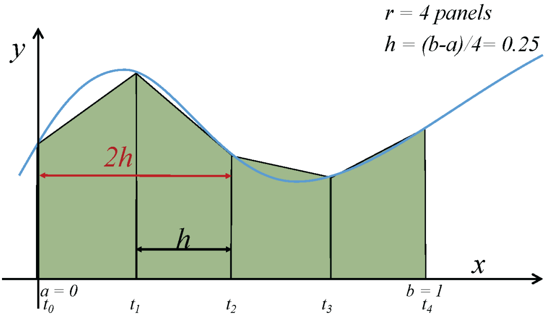

Figure 2

(cont.)

Recall Simpson's rule:

$$I(f) = \frac{b-a}{6}[f(x_0) + 4f(x_1) + f(x_2)],$$

which we can apply to each one of the two sub-intervals, $[t_0, t_2]$ and $[t_2, t_4]$.

Let's call the integrals over the two sub-intervals, S_1 and S_2 :

$$S_1 = \frac{t_2 - t_0}{6}[f(t_0) + 4f(t_1) + f(t_2)],$$
$$S_2 = \frac{t_4 - t_2}{6}[f(t_2) + 4f(t_3) + f(t_4)].$$

(cont.)

The total integral is then just the sum of these two. Here notice that each sub-interval is of length $2h$, allowing us to simplify the sums.

$$\begin{aligned} I(f) = \ S_1 + S_2 = \ & \frac{h}{3}[f(t_0) + 4f(t_1) + f(t_2)] + \\ & \frac{h}{3}[f(t_2) + 4f(t_3) + f(t_4)]. \end{aligned}$$

Now, rearranging the terms we get:

$$\begin{aligned} I_{Simp}(f) &= \frac{h}{3}[f(t_0) + 4f(t_1) + 2f(t_2) + 4f(t_3) + f(t_4)], \\ &= \frac{h}{3}[f(t_0) + 4[f(t_1) + f(t_3)] + 2f(t_2) + f(t_4)]. \end{aligned}$$

Looking closely, one can start to see a general pattern:

Important

! Important

An important consequence of this approach is that ***the quadrature formulas lose one order of*** h ***in their approximations.***

- Even though each individual panel has the original truncation error, when we add up all the panels, the errors from each of the individual panels add up and we lose one order of magnitude.
- However, since h is smaller, the overall result is a win!

Section 2

Error Analysis

Error Analysis and Stability

- While we have a fairly good handle on the error analysis of quadrature formulas and the order of convergence, one question we haven't addressed yet is the stability of quadrature formulas.
- First, we know that the truncation error is well-behaved and will go to zero at varying degrees depending on the degree of the interpolating polynomial we use.
- What caused problems before was that roundoff error could increase dramatically leading to unstable algorithms.

(cont.)

- Let's proceed as before, by performing a floating point error analysis similar to the one we used for numerical differentiation.
- Recall, that we first assumed that a computation of a function value always incurs some roundoff error, in other words, we can write:

$$f(t_i) = \hat{f}(t_i) + e_i,\ i = 0, 1, \ldots, n,$$

where $\hat{f}$ is the floating point representation and e_i is the roundoff error incurred when computing the function value. - As before, we will assume that the errors are uniformly bounded:

$$e_i < \epsilon, \quad \epsilon > 0, \quad \forall\ i$$

(cont.)

If we substitute into the Composite Simpson's rule we can write the error as:

$$
\begin{aligned}
|e(h)| &= \Big|\frac{h}{3}(e_0 + 2\sum_{i=1}^{r/2-1} e_{2i} + 4\sum_{i=1}^{r/2} e_{2i-1} + e_r)\Big|, \\
&\leq \frac{h}{3}(\epsilon + 2(\frac{r}{2} - 1)\epsilon + 4(\frac{r}{2})\epsilon + \epsilon), \\
&\leq \frac{h}{3}(3r\epsilon) = rh\epsilon.
\end{aligned}
$$

(cont.)

Finally, let's remember that $h = (b - a)/r$, which means that the error is bounded by:

$$|e(h)| \leq (b - a)\ \epsilon,$$

which is independent of both h and r.

Important

In other words, Simpson's rule is stable!

Furthermore, it should be obvious that we can do the same analysis for any of the open or closed Newton-Cotes quadrature formulas. Unlike numerical differentiation, quadrature is generarlly more stable.

Exercise

Exercise

Determine values of h that will ensure an approximation error of < 0.00002 when approximating

$$\int_0^{\pi} \sin x dx$$

using

1. Composite Trapezoidal Rule
2. Composite Simpson's Rule

Solution

Composite Trapezoid. Our starting point is the formula for the truncation error. For composite Trapezoid we use Equation 1:

$$E(f) = -\frac{b-a}{12}h^2 f''(\xi).$$

We would like this term to be less than the tolerance $\epsilon = 2 \cdot 10^{-5}$

$$\begin{aligned} |E(f)| &= \left|\frac{\pi}{12}h^2 \sin(\xi)\right| \\ &= \frac{\pi}{12}h^2 \left|\sin(\xi)\right| \\ &\leq \frac{\pi h^2}{12} < 2 \cdot 10^{-5} \end{aligned}$$

with the last inequality because $|\sin(x)| \leq 1$.

(cont.)

Solving for h is then an easy matter:

$$\begin{aligned}
\frac{\pi h^2}{12} &< 2 \cdot 10^{-5}, \\
h^2 &< \frac{24 \cdot 10^{-5}}{\pi}, \\
h &< \sqrt{\frac{24 \cdot 10^{-5}}{\pi}}. \\
\implies h &\approx 0.00874.
\end{aligned}$$

To achieve the desired accuracy, would then require $r = (b - a)/h$ panels or $r \approx 360$ panels.

Composite Simpson

Composite Simpson. As before, our starting point is the formula for the truncation error. For composite Simpson we use Equation 2:

$$E(f) = -\frac{b-a}{180} h^4 f^{(4)}(\xi).$$

We would like this term to be less than the tolerance $\epsilon = 2 \cdot 10^{-5}$

$$\begin{aligned} |E(f)| &= \left| \frac{\pi}{12} h^4 \sin(\xi) \right|, \\ &= \frac{\pi}{12} h^4 \left| \sin(\xi) \right|, \\ &\leq \frac{\pi h^4}{180} < 2 \cdot 10^{-5}, \end{aligned}$$

with the last inequality because $|\sin(x)| \leq 1$.

(cont.)

Solving for h:

$$
\begin{aligned}
\frac{\pi h^4}{180} &< 2 \cdot 10^{-5}, \\
h^4 &< \frac{360 \cdot 10^{-5}}{\pi}, \\
h &< \sqrt[4]{\frac{360 \cdot 10^{-5}}{\pi}}. \\
\implies h &\approx 0.18399
\end{aligned}
$$

To achieve the desired accuracy, would then require $r = (b-a)/h$ panels or $r \approx 18$ panels. For this example, it is clear that Composite Simpson is a much better choice than Composite Trapezoid.

Section 3

Summary

Summary

- There are several choices to be made when considering which quadrature method to use and what size of h to choose.
- Deciding between a lower order method versus a higher order method can also be tricky.
- The error term will depend on both the size of h as well as the magnitude of the highest derivative required.
- Choosing h will require (as in the case of numerical differentiation) a balance between truncation error and roundoff error.

Practical Tips

Choosing a quadrature method and h

1. The smaller h is, the greater the accuracy for all methods; however that also implies we have more panels and hence a higher computational load.
2. If the function that is to be integrated is smooth then higher order methods are likely to work well.
3. However, if the the function is rapidly changing, then the higher derivatives will likely be large and one might want to consider lower order methods, especially if the integral interval is small.