Numerical Integration Basics

Math 131: Numerical Analysis

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Section 1

Introduction

Motivation

What is the first thing you think of when you see:

$$\int_a^b f(x)dx \tag{1}$$

This leads us to the **general strategy**:

Approximate

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

for some yet to be determined coefficients a_i.

We will call this ***numerical quadrature***.

Approach

To do this we will follow the same strategy we used for numerical differentiation, i.e. we will replace the function whose integral we seek with one whose integral can be more easily evaluated – an *interpolating polynomial*.

Our overall goal is to approximate the integral in Equation 1 by computing $\sum_{i=0}^{n} a_i f(x_i)$ through the following 3 steps:

1. Approximate $f(x)$ by an interpolating polynomial
2. Integrate the polynomial
3. Understand/analyze the truncation error

Intuition

Before we start, let's first develop some intuition on what we're doing. Consider Figure 1 in which we've plotted a generic function. A natural idea is to use the well-known trapezoidal rule to approximate the area under the curve.

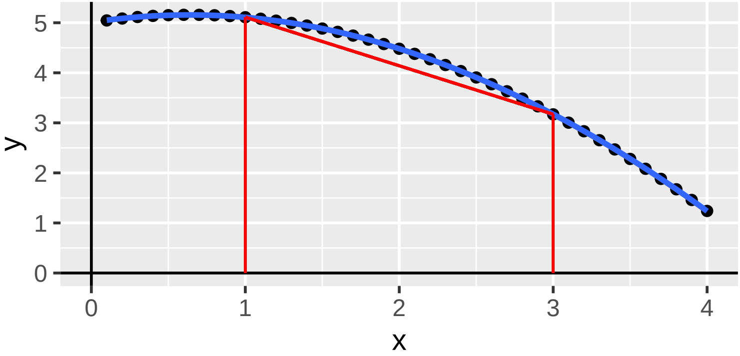

Figure 1: Trapezoidal Rule.

(cont.)

If we do this, it would make sense to approximate the integral as:

$$\int_1^3 f(x)dx \approx \frac{h}{2}[f(x_0) + f(x_1)],\ x_0 = 1, x_1 = 3,$$

where h is defined as the interval width, i.e. $h = b - a = 3 - 1$.

Notice also, that in Figure 1 all that we did was to approximate the function by using a linear approximation using the two endpoints.

It is natural to conjecture for what type of functions would the trapezoidal rule be exact for? Can you guess?

Remarks

- In order to get a more accurate approximation, we could subdivide the total region into smaller trapezoids and sum over all of them.
- To make this more rigorous we will need to develop our framework and compute error estimates for our approximations.
- We will return to this idea in our lectures on **Composite Integration**

Section 2

Interpolating Polynomials

Step 1. Write down our function as a Lagrange interpolating polynomial along with its truncation error.

Let

$$f(x) = \sum_{i=0}^{n} f(x_i) L_i(x) + \prod_{i=0}^{n} (x - x_i) \frac{f^{(n+1)}(\xi(x))}{(n+1)!}. \tag{2}$$

For convenience, let's denote

$$\Psi_n(x) = \prod_{i=0}^{n} (x - x_i).$$

We can then write Equation 2 as:

$$f(x) = \sum_{i=0}^{n} f(x_i) L_i(x) + \Psi_n(x) \ \frac{f^{(n+1)}(\xi(x))}{(n+1)!}.$$

Interpolating Polynomials

Step 2. Integrate the interpolating polynomial:

$$\int_a^b f(x) = \int_a^b \sum_{i=0}^{n} f(x_i)L_i(x) + \int_a^b \Psi_n(x)\ \frac{f^{(n+1)}(\xi(x))}{(n+1)!}.$$

Notice we can move the integral under the sum for the first term. Now (again for convenience) let's denote

$$a_i = \int_a^b L_i(x)dx,\ i = 0, \ldots, n. \tag{3}$$

(cont.)

Rearranging we get:

$$\int_a^b f(x) = \sum_{i=0}^{n} a_i f(x_i) + E(f),$$

where we denote the truncation error $E(f)$ by:

$$E(f) = \frac{1}{(n+1)!} \int_a^b \Psi_n(x)\ f^{(n+1)}(\xi(x))dx. \tag{4}$$

Notice we are partway to our goal of having written down the integral in the form we wanted:

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

Example: Linear Interpolating Polynomial

Specific Case: $n = 1$ **(Linear Interpolating Polynomial)**

Let's take the easiest case, $n = 1$, a linear Lagrange interpolating polynomial. To be consistent with our earlier notation we'll also let $a = x_0$ and $b = x_n = x_1$ for this case.

Recall, the first degree Lagrange polynomial takes the form:

$$P_1(x) = \frac{(x - x_1)}{x_0 - x_1} f(x_0) + \frac{(x - x_0)}{x_1 - x_0} f(x_1), \tag{5}$$

and the truncation error Equation 4 reduces to

$$E(f) = \frac{1}{2} \int_{x_0}^{x_1} (x - x_0)(x - x_1) f''(\xi(x)) dx. \tag{6}$$

Remaining Steps

We're now left with only two steps:

2. Compute a_i for a specific interpolating polynomial, and
3. Understand/analyze the error function $E(f)$

Let's take these one at a time

Section 3

Computation of the Integrals

Compute the integrals

Let's consider the second step where we need to compute the integrals of Equation 5, i.e.

$$\int_{x_0}^{x_1} P_1(x) = \int_{x_0}^{x_1} \frac{(x - x_1)}{x_0 - x_1} f(x_0) + \frac{(x - x_0)}{x_1 - x_0} f(x_1),$$
$$= \left[\frac{(x - x_1)^2}{2(x_0 - x_1)} f(x_0) + \frac{(x - x_0)^2}{2(x_1 - x_0)} f(x_1) \right]_{x_0}^{x_1}.$$

Notice that for the upper value x_1 the first term in the sum drops out, and likewise for the lower value x_0 the second term drops out, leaving only 2 terms.

(cont.)

Evaluating these two terms we get:

$$\begin{aligned}
\int_{x_0}^{x_1} P_1(x) &= \left[\frac{(x_1-x_0)^2}{2(x_1-x_0)} f(x_1) - \frac{(x_0-x_1)^2}{2(x_0-x_1)} f(x_0)\right], \\
&= \left[\frac{(x_1-x_0)}{2} f(x_1) - \frac{(x_0-x_1)}{2} f(x_0)\right], \\
&= \left[\frac{(x_1-x_0)}{2} f(x_1) + \frac{(x_1-x_0)}{2} f(x_0)\right], \\
&= \left(\frac{x_1-x_0}{2}\right) \left[f(x_1) + f(x_0)\right], \\
&= \frac{h}{2} \left[f(x_1) + f(x_0)\right],
\end{aligned}$$

where the last line is due to the fact that $x_1 = x_0 + h$.

Trapezoidal Rule

This leads us to the well-known Trapezoidal Rule:

Trapezoidal Rule

$$\int_a^b f(x)dx \approx \frac{h}{2}\left[f(x_0) + f(x_1)\right].$$

Section 4

Error Analysis

Step 3 - Understand/Analyze the Truncation Error

Recall: the truncation error (Equation 6) was given by:

$$E(f) = \frac{1}{2} \int_{x_0}^{x_1} (x - x_0)(x - x_1) f''(\xi(x)) dx.$$

- It would be nice if we could take $f''(\xi(x))$ term outside the integral to simplify the integral.
- Let's first define $g(x) = (x - x_0)(x - x_1)$, and notice that $g(x)$ doesn't change sign on $[x_0, x_1]$.
- That means we can apply the Weighted Mean Value Theorem (WMVT) for integrals and pull the $f''(\xi(x))$ term outside of the integral.

Recall WMVTI

Weighted Mean Value Theorem for Integrals:

Suppose that $f \in C[a,b]$, the Riemann integral of g exists on $[a,b]$, and $g(x)$ does not change sign on $[a,b]$. Then there exists a number $c \in (a,b)$ such that

$$\int_a^b f(x)g(x)dx = f(c)\int_a^b g(x)dx$$

Using WMVTI

That simplifies $E(f)$ so that

$$E(f) = \frac{1}{2} f''(\xi) \int_{x_0}^{x_1} (x - x_0)(x - x_1) dx,$$

for some $\xi \in [x_0, x_1]$.

Integrating the quadratic

That just leaves us with integrating the quadratic inside the integral, which reduces to:

$$E(f) = \frac{1}{2} f''(\xi) \left[\frac{x^3}{3} - \frac{(x_1 + x_0)}{2} x^2 + x_0 x_1 x \right]_{x_0}^{x_1}. \tag{7}$$

To simplify the calculations, let's first do a change of variable, $x' = x - x_0$. Also recall that $x_1 = x_0 + h$.

With the change of variable, the limits reduce to $x_0 \to 0, x_1 \to h$, and

$$E(f) = \frac{1}{2} f''(\xi) \left[\frac{x^3}{3} - \frac{(x_1 + x_0)}{2} x^2 + x_0 x_1 x \right]_{0}^{h}. \tag{8}$$

(cont.)

As a result, the term in brackets in Equation 8 evaluates to:

$$\left[\frac{h^3}{3} - \frac{(h)h^2}{2} + 0\right] = \frac{-h^3}{6}.$$

This gives us the following form for $E(f)$

$$E(f) = -\frac{h^3 f''(\xi)}{12}.$$

That takes care of Step 3 - Understand/Analyze the Truncation Error $E(f)$!

Trapezoidal Rule

Pulling it all together, this leads us to our desired result:

Trapezoidal Rule with Error Term

$$\int_a^b f(x)dx = \frac{h}{2}\left[f(x_0) + f(x_1)\right] - \frac{h^3}{12} f''(\xi),$$

Since the truncation error is given by $\frac{h^3}{12} f''(\xi)$ we expect that for ***any function whose second derivative is identical to zero that the Trapezoidal Rule will be exact***, and in particular for any polynomial of degree 1 or less.

Section 5

Simpson's Rule

Note

Note

The derivation for Simpson's Rule follows the one for the Trapezoidal Rule, with some minor modifications. The following is included for completeness (and for practice), but you may also want to skip down to the final formula (Equation 13) and discussion of the major properties of Simpson's Rule.

Simpson's Rule

In a similar fashion to our approach for deriving the Trapezoid Rule, if we integrate the second-degree Lagrange polynomial, we can derive Simpson's Rule.

Conjecture

1. For what degree polynomials will Simpson's rule be exact?
2. What do you think the order of the truncation error will be for Simpson's method?

Setting up the integral of the interpolating polynomial.

As before, we will first approximate the integrand by an interpolating polynomial. In this case we will take 3 equally spaced points x_0, x_1, x_2 such that $x_0 = a, x_1 = x_0 + h, x_2 = b$, where $h = (b-a)/2$.

We assumed that $f(x)$ had as many derivatives as we needed. This time let's write the Taylor expansion for $f(x)$ about x_1 going out to the 4th derivative term. The reason for going out to the 4th derivative will become clear in a minute.

$$\begin{aligned} f(x) = f(x_1) + f'(x_1)(x - x_1) + \frac{1}{2} f''(x_1)(x - x_1)^2 \\ + \frac{1}{6} f'''(x_1)(x - x_1)^3 + \frac{1}{24} f^{(4)}(\xi), \qquad \xi \in [x_0, x_2] \end{aligned}$$

(cont.)

Now let's integrate this equation:

$$\int_{x_0}^{x_2} f(x) = \Big[f(x_1)(x - x_1) + \frac{1}{2} f'(x_1)(x - x_1)^2 + \frac{1}{6} f''(x_1)(x - x_1)^3 + \frac{1}{24} f'''(x_1)(x - x_1)^4 \Big]_{x_0}^{x_2} + \frac{1}{24} \int_{x_0}^{x_2} f^{(4)}(\xi(x))(x - x_1)^4 dx. \tag{9}$$

(cont.)

Let's consider the error term first and notice that it would be nice to take the $f^{(4)}(\xi(x))$ in the last term outside of the integral.

Using the previous trick, we note that $(x - x_1)^4$ doesn't change sign in the interval $[x_0, x_1]$, so we can again use the Weighted Mean Value Theorem for Integrals to pull the $f^{(4)}$ term out from inside the integral.

$$\begin{aligned} E(f) &= \frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi(x))(x - x_1)^4 dx, \\ &= \frac{f^{(4)}(\xi_1)}{24}\int_{x_0}^{x_2}(x - x_1)^4 dx, \\ &= \frac{f^{(4)}(\xi_1)}{120}(x - x_1)^5\Big|_{x_0}^{x_2}. \end{aligned}$$

for some $\xi_1 \in [x_0, x_2]$.

(cont.)

Now we can use the fact that $h = x_2 - x_1 = x_1 - x_0$ to reduce the equation to:

$$E(f) = \frac{h^5 f^{(4)}(\xi_1)}{60}. \tag{10}$$

Evaluating the integral of the interpolating polynomial.

Our only remaining task is to evaluate the first term in Equation 9 to produce the approximation for $I(f)$. :

$$\Big[f(x_1)(x - x_1) + \frac{1}{2} f'(x_1)(x - x_1)^2 \\ + \frac{1}{6} f''(x_1)(x - x_1)^3 + \frac{1}{24} f'''(x_1)(x - x_1)^4 \Big]_{x_0}^{x_2}$$

(cont.)

Recall that $x_2 - x_1 = x_1 - x_0 = h$ – which reduces our formula to:

$$\left[f(x_1)h + \frac{1}{2}f'(x_1)h^2 + \frac{1}{6}f''(x_1)h^3 + \frac{1}{24}f'''(x_1)h^4\right] -$$
$$\left[f(x_1)(-h) + \frac{1}{2}f'(x_1)h^2 + \frac{1}{6}f''(x_1)(-h)^3 + \frac{1}{24}f'''(x_1)h^4\right].$$

Nicely, the h^2 and h^4 terms cancel out, leaving us with

$$2hf(x_1) + \frac{h^3}{3}f''(x_1). \tag{11}$$

Tip

We could just as easily have noticed that (under the assumption of equally spaced nodes), $(x_2 - x_1)^k - (x_0 - x_1)^k = 0$ for even k and that $(x_2 - x_1)^k - (x_0 - x_1)^k = 2h^k$ for odd k.

(cont.)

Now remember our goal was to write our approximation in terms of only $f(x_i)$, meaning we should look for a way to replace the second derivative term in Equation 11.

For this task, we can take advantage of one last substitution, which is to use our finite difference approximation for the second derivative (derived in our previous lecture), i.e.

$$f''(x_1) = \frac{f(x_0) - 2f(x_1) + f(x_2)}{h^2} - \frac{h^2}{12} f^{(4)}(\xi_2)$$

and not forgetting to include its own error term.

(cont.)

When we substitute the second derivative approximation into Equation 11 we get:

$$2hf(x_1) + \frac{h^3}{3}\left[\frac{f(x_0) - 2f(x_1) + f(x_2)}{h^2} - \frac{h^2}{12}f^{(4)}(\xi_2)\right] \tag{12}$$

Combining Equation 12 with Equation 10 and simplifying terms we arrive at our final result, which is called Simpson's Rule:

Simpson's Rule

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90}f^{(4)}(\xi). \tag{13}$$

Exercise: combining the two derivative terms

I leave as an exercise how to combine the two $f^{(4)}$ terms from Equation 10 and Equation 12 into one, i.e. show that

$$-\frac{h^5}{60}f^{(4)}(\xi_1) - \frac{h^5}{36}f^{(4)}(\xi_2) = -\frac{h^5}{90}f^{(4)}(\xi), \quad \xi \in (a,b)$$

Remarks

Note

Other formulas use $\frac{b-a}{6}$ instead of $\frac{h}{3}$ in the definition of Simpson's Rule. Just remember that here, we defined $h = x_2 - x_1 = x_1 - x_0$, so $h = \frac{b-a}{2}$, as a result the two definitions are equivalent.

An important result is that instead of the expected $O(h^4)$ error term, we might have expected from going from a linear interpolant to a quadratic interpolant we have instead ***gained an additional order of accuracy*** in the error term!

Precision

Definition

Definition: The ***precision*** (also degree of accuracy) of a quadrature formula is defined as the largest positive integer n such that the quadrature formula is exact for x^k, for $k = 0, 1, \ldots, n$.

- In the case of Simpson's rule, it is exact for any polynomial of degree 3 or less, hence the precision is 3.
- Similarly, the precision for the Trapezoid rule is 1. The easiest way to remember this is to take a look at the derivative in the error term and subtract one order.
- Please do not confuse this with the order of accuracy, which can be seen from the power in the h term!

Section 6

Summary

Summary

- Introduced the concepts of numerical integration
- Derived the Trapezoidal and Simpson's rule using interpolating polynomials
- Introduced the notion of precision of quadrature rules:
  - Trapezoid has precision 1
  - Simpson's rule has precision 3

Newton-Cotes

Math 131: Numerical Analysis

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Section 1

Introduction

Recall

Approximate

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

General approach was to approximate the integral by:

1. Approximate $f(x)$ by an interpolating polynomial
2. Integrate the polynomial

Recall (cont.)

Trapezoidal Rule

$$\int_a^b f(x)dx \approx \frac{h}{2}\left[f(x_0) + f(x_1)\right].$$

where $h = b - a, x_0 = a, x_1 = b$.

Simpson's rule

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)]. \tag{1}$$

where $h = (b-a)/2, x_0 = 1, x_1 = (a+b)/2, x_2 = b$

Section 2

Exercise

Exercise

Exercise

Compute the value of

$$\int_0^1 e^x dx$$

using the Trapezoid and Simpson's Rule for:

1. $a = 0$, $b = 1$
2. $a = 0.9$, $b = 1$

What is the error in each case?

Trapezoid Rule

Trapezoid Rule:

$$\int_a^b f(x)dx = \frac{(b-a)}{2}\Big[f(x_0) + f(x_1)\Big],$$

Simpson's Rule:

$$\int_a^b f(x)dx = \frac{(b-a)}{6}[f(x_0) + 4f(x_1) + f(x_2)]$$

Remarks

- Notice that both formulas have a rather large error when we compute the integral over a “large” interval,
- Whereas when we considered a smaller interval, the error was in fact quite small.
- How can we get better estimates?

Section 3

Higher-Order Methods

Newton-Cotes

- The basic quadrature rules derived so far are generally good, but what if we wanted to have formulas with greater accurarcy.
- The general approach we used still holds and leads to a family of quadrature formulas known as ***Newton-Cotes*** formulas.
- These are classified under either open or closed depending on whether the formulas include the end points or not.
  - ***Closed Newton-Cotes*** include the endpoints of closed interval $[a, b]$ as nodes.
  - ***Open Newton-Cotes*** do not include the endpoints.

In particular

To be specific, for a ***closed*** Newton-Cotes quadrature formula we would choose the node points x_i through the formula:

$$x_i = a + i\frac{b-a}{n-1}, \quad i = 0, 1, \dots, n-1. \tag{2}$$

For an ***open*** Newton-Cotes quadrature formula we would use the formula:

$$x_i = a + (i+1)\frac{b-a}{n+1}, \quad i = 0, 1, \dots, n-1. \tag{3}$$

Example

Suppose, we choose $n = 5$ on the interval [a,b] $=$ [0,1].

Then Equation 2 (closed) would generate the points:

$$\begin{aligned} x_i &= a + i \ \cdot \frac{b-a}{n-1}, \\ &= 0 + i\frac{1}{4}, \\ &= \frac{i}{4}, \quad i = 0, 1, \ldots, 4, \end{aligned}$$

thereby yielding the set of nodes: $\{x\} = \{\ 0, .25, .5, .75, 1.0\ \}$.

Example

Similarly Equation 3 (open) would generate the points:

$$
\begin{aligned}
x_i &= a + (i+1) \cdot \frac{b-a}{n+1}, \\
&= 0 + (i+1)\frac{1}{6}, \\
&= \frac{i+1}{6}, \quad i = 0, 1, \dots, 4,
\end{aligned}
$$

which generates the set of nodes:

$$\{x\} = \{\ 1/6,\ 2/6,\ 3/6,\ 4/6,\ 5/6\ \}.$$

Some previous examples

- One example of an Open Newton-Cotes is the midpoint rule

$$\int_a^b f(x)dx = 2hf(x_0) + \frac{h^3}{3}f''(\xi)\ \xi \in (a,b)]$$

where x_0 is the midpoint between a and b.

- Likewise, both Trapezoidal and Simpson's rules can be categorized as Closed Newton-Cotes.

Other formulas

- There are many different formulas of both the Closed and Open variety all with corresponding error terms.
- All of them can be derived by the methods we've used for Trapezoid and Simpson's rule, so there is little to be gained by re-deriving them.
- Instead we will present them here because an interesting pattern arises that is worth knowing about:

Closed Newton-Cotes formulas:

$n = 2$ (Trapezoid)

$$I(f) = \frac{b-a}{2}[f(x_0) + f(x_1)] \tag{4}$$

$n = 3$ (Simpson's)

$$I(f) = \frac{b-a}{6}[f(x_0) + 4f(x_1) + f(x_2)] \tag{5}$$

$n = 4$ (Simpson's 3/8)

$$I(f) = \frac{b-a}{8}[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)] \tag{6}$$

$n = 5$ (Boole's rule)

$$I(f) = \frac{b-a}{90}[7f(x_0) + 32f(x_1) + 12f(x_2) + 32f(x_3) + 7f(x_4)] \tag{7}$$

Trip-Hazard - Notation

- The formulas here are written using $b - a$ versus h to make them easier to compare.
- However, you will see these formulas written in terms of h in many other places.
- You should be careful in understanding exactly what h represents as it often is taken to mean $h = (b-a)/(n-1),\ n \geq 1$, which is related to the number of node points used in the quadrature formula.

Higher-order formulas

- In theory, we could go as high as we wanted (and people have) in generating higher-order quadrature formulas, and of course with additional computational work.
- However, for large n the formulas can be shown to become numerically unstable $(n \geq 11.)$ One can actually prove that formulas do not converge for all integrands that are analytic.
- In practice, we tend to only use low-order formulas since they can still give us good accuracy (especially over small intervals (see Exercise 2.1 below).

Open Newton-Cotes formulas:

$n = 1$ (Midpoint)

$$I(f) = (b-a)f(x_0) \tag{8}$$

$n = 2$

$$I(f) = \frac{b-a}{2}[f(x_0) + f(x_1)] \tag{9}$$

$n = 3$

$$I(f) = \frac{b-a}{3}[2f(x_0) - f(x_1) + 2f(x_2)] \tag{10}$$

Similarly to the closed Newton-Cotes formulas, we could continue and derive higher-order formulas - with the same consequences.

Section 4

Error Estimates

Error Estimates

In both the closed and open Newton-Cotes cases, the formulas have error terms, which we have summarized in the table below, along with the precision of each:

Table 1: Summary of Error Terms for Newton-Cotes quadrature formulas

Name	N (npts)	Error	Precision
Trapezoid	2	$-\frac{(b-a)^3}{12} f^{(2)}(\xi)$	1
Simpson's	3	$-\frac{(b-a)^5}{2880} f^{(4)}(\xi)$	3
Simpson's 3/8	4	$-\frac{(b-a)^5}{6480} f^{(4)}(\xi)$	3
Boole	5	$-\frac{(b-a)^7}{1935360} f^{(6)}(\xi)$	5
Midpoint	1	$\frac{(b-a)^3}{24} f^{(2)}(\xi)$	1
	2	$\frac{(b-a)^3}{36} f^{(2)}(\xi)$	1
	3	$\frac{(b-a)^5}{23040} f^{(4)}(\xi)$	3

Remarks

Important

- An interesting feature of the quadrature formulas is that whenever N is odd then the precision of the formula $= N$.
- But when N is even then the precision is only $N - 1$.
- We lose one order in the precision whenever N is even! Or we could also say that we gain one order of precision for N odd.

Section 5

Summary

Summary

- A simple approach towards deriving basic quadrature rules is to replace the integrand with an interpolating polynomial on a chosen set of points and integrate the polynomial.
- Taylor's theorem yield error terms that provide us with estimates on how well the quadrature formula approximates the integral.
- The precision of a quadrature formula is the highest degree of the polynomial for which the formula is exact. When N is odd, the precision is also N; but when N is even, the precision is $N - 1$.
- Higher-order formulas yield greater accuracy, but at greater computational work as well as a fundamental assumption that the higher-order derivatives are nicely behaved (i.e. bounded).
- Basic (low-order) formulas can be accurate, but usually require a small interval. This observation will prove useful in the next sections.

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

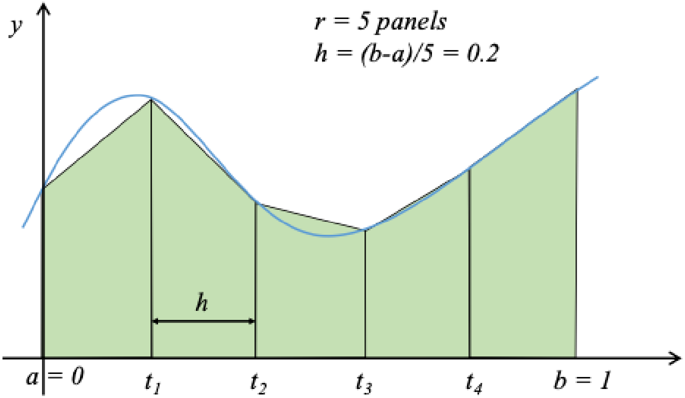


Figure 1: Approximating the integral by sudviding the region into multiple "panels" and using the trapezoid rule will lead to higher accuracy

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 $t_i = a + ih,\ i = 0, \ldots, r,\ h = (b - a)/r$.

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

Section 2

Example (Trapezoid Rule)

Example

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

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

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

Caution

Notice that the error term loses one order in h. More on this in a minute.

Section 3

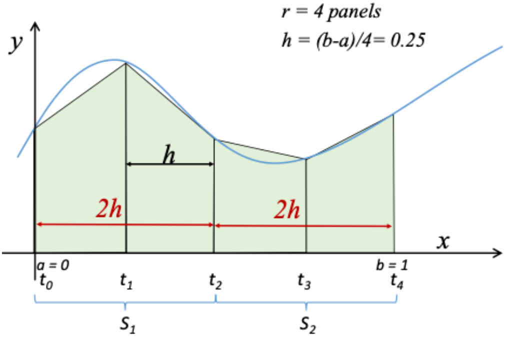
Example (Simpson's Rule)

Composite Simpson's Rule

- 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.***

Simpson's rule - 4 panels

- 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 $[t_2, t_4]$.



(cont.)

First 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 :

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

Note: $t_2 - t_0 = t_4 - t_2 = 2h.$

(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. This leads to the Composite Simpson's Rule formula:

Composite Simpson's

Composite Simpson's Rule

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

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

Caution

As with Composite Trapezoid the error term loses one order in h.

Composite Rules' Error Terms

! Important

An important consequence of using composite rules 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!

Sketch of proof:

$$E = \sum_{i=1}^{r} -\frac{h^5}{90} f^{(4)}(\xi_i) = C \sum_{i=1}^{r} h^5, = C \cdot rh^5,$$
$$= C \frac{(b-a)}{h} h^5 = C(b-a)h^4.$$

Section 4

Stability and Error Analysis

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 algorithms.
- 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 in numerical differentiation was that roundoff error could increase dramatically leading to unstable algorithms.

Roundoff Error Analysis

- 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:

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

(cont.)

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

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

(cont.)

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

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

which is independent of both h and r. Of course, the bigger the interval the bigger the bound.

We can do the same analysis for any of the open or closed Newton-Cotes quadrature formulas.

Important

Unlike numerical differentiation, ***Simpson's rule is stable!***

Section 5

Choosing good values of h

Choosing h to achieve given tolerance

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:

$$E(f) = -\frac{b-a}{12}h^2 f''(\mu), \quad \mu \in [a, b]$$

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

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

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 $r \approx (\pi - 0)/0.00874 \approx 360$ panels.

Solution (cont.)

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

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

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

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

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 6

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 - Composite Quadrature

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 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.

Adaptive Quadrature

Math 131: Numerical Analysis

J.C. Meza

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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:

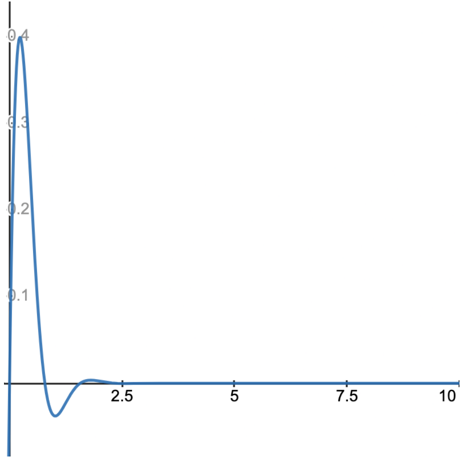

Figure 1: $f(x) = e^{-3x}\sin(4x),\ x \in [0, 10]$

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

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

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.