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.

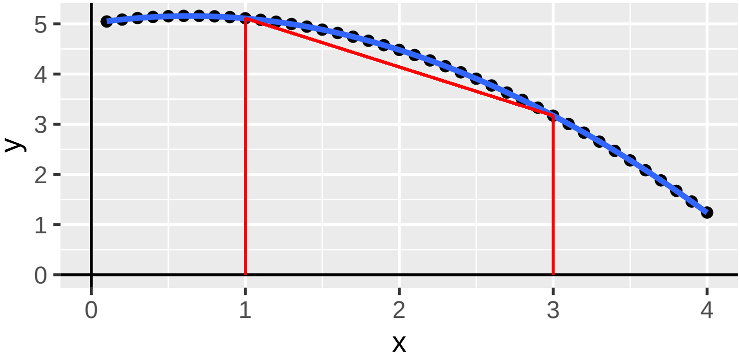

Figure 1: Trapezoidal Rule.

(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

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

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.

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

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.

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

(cont.)

Now let's integrate this equation:

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

(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:

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

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

Simpson's Rule

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

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