1 Numerical Integration

Recall that last lecture, we discussed numerical integration. Given an interval $[a, b]$ and a function $f : [a, b]$, we would like to find the area under the curve over $[a, b]$, I:
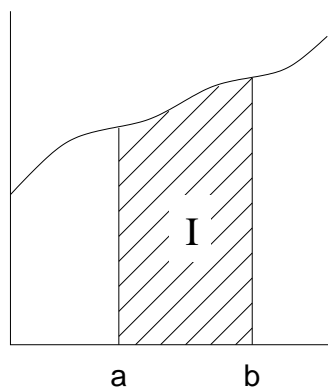
$$I \;=\; \int_a^b f(t)dt$$

as shown in Figure 1.

Figure 1: The Definite Integral of $f(t)$ over $[a, b]$

Recall from the fundamental theorem of calculus that we can find I using the antiderivative, a function F with $F' = f$

$$I \;=\; F(b) - F(a)$$

However, as we discussed last lecture, this method is nearly useless in numerical integration except in very special cases (such as integrating polynomials). To illustrate, consider the following example:

EXAMPLE 1.1. *Find the numerical value of* $\log(1.2)$. *We recall that the natural log is defined using the definite integral of a simple, rational function, as shown in Figure 2:*

$$\log(x) \;=\; \int_1^x \frac{1}{t}dt \quad \text{and thus}$$
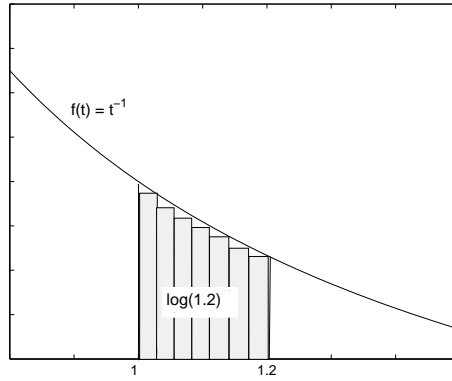$$\log(1.2) \;=\; \int_1^{1.2} \frac{1}{t}dt$$

Figure 2: Calculating the Natural Logarithm with a Definite Integral

So, if we can find a method to give a numerical approximation of definite integrals, we can use it to find numerical approximations of the natural log.

Many functions don't even have antiderivatives expressible in terms of simple functions like cos, exp, etc. One important example is

$$\int_a^b e^{-t^2} dt$$

2   Basic Rules for Numerical Approximation of Definite Integrals

All of the basic methods for numerical approximation that we will examine rely on the same basic idea:

1. Approximate $f|_{[a,b]}$ using some polynomial p

2. Integrate the polynomial:

$$I_{\text{rule}} \;\; = \;\; \int_a^b p(t)\mathrm{dt} \approx \int_a^b f(t)\mathrm{dt}$$

Suppose that we obtain the approximating polynomial p through interpolation. Given $n+1$ nodes $[t_0, t_1, \ldots, t_n]$, we can write p using the Lagrange representation:

$$p(t) \;\; = \;\; f(t_0) \cdot \ell_0(t) + f(t_1) \cdot \ell_1(t) + \cdots + f(t_n) \cdot \ell_n(t)$$

Integrating this polynomial, we get our approximation of $f|_{[a,b]}$:

$$I_{\text{rule}} \quad = \quad \int_a^b p(t)\mathrm{dt} \tag{1}$$

$$= \quad \int_a^b \sum_{i=0}^{n} f(t_i) \cdot \ell_i(t)\mathrm{dt} \tag{2}$$

$$= \quad \sum_{i=0}^{n} \left(f(t_i) \cdot \underbrace{\int_a^b \ell_i(t)\mathrm{dt}}_{w_i} \right) \tag{3}$$

Where w_i is a *weight* applied to each function value. Note that, since Lagrange polynomials do not depend on the function, we can calculate the weights w_i using only the nodes $[t_0, t_1, \ldots, t_n]$, thus we can rewrite equation 3 as a simple weighted sum of function values:

$$I_{\text{rule}} \quad = \quad \sum_{i=0}^{n} f(t_i) \cdot w_i \tag{4}$$

Now we will discuss four simple rules that follow this general framework.

2.1 Rectangle Rule

In the *rectangle rule*, we approximate $f|_{[a,b]}$ using a single interpolation point $[a]$ (the left endpoint of the interval). Our polynomial interpolant will thus be a constant polynomial $p(t) = f(a)$, as shown in Figure 3 and we can calculate its area I_R using:

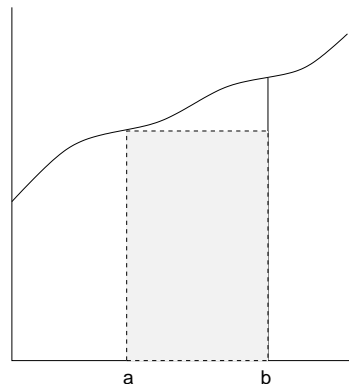$$I_R \quad = \quad f(a) \cdot (b - a) \tag{5}$$

Figure 3: The Rectangle Rule for Approximating a Definite Integral

Approximating the solution to example 1.1 using the rectangle rule yields:

$$\begin{aligned}
I &= \int_1^{1.2} \frac{1}{t}\mathrm{dt} \\
&\approx I_R \\
&= f(1) \cdot (1.2 - 1) \\
&= \frac{1}{1} \cdot 0.2 \\
&= 0.2
\end{aligned}$$

We can summarize the rectangle rule by the notation

$$\{a\}$$

This notation means that the rectangle rule approximates the integral $\int_a^b f(t)\,dt$ by evaluating f at a, finding the polynomial which interpolates the point $(a, f(a))$, and integrating this polynomial.

2.2 Midpoint Rule

In the *midpoint rule*, we again approximate $f|_{[a,b]}$ using a single interpolation point, but this time we use the midpoint $\frac{a+b}{2}$. Our polynomial interpolant will again be a constant polynomial, this time $p(t) = f\left(\frac{a+b}{2}\right)$, as shown in Figure 4 and we can calculate its area I_M using:

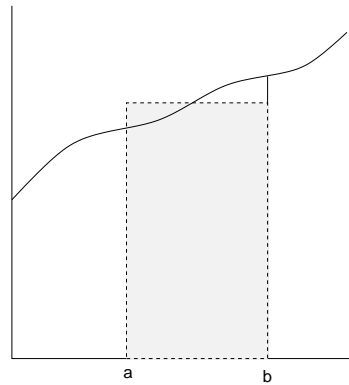$$I_M = f\left(\frac{a+b}{2}\right) \cdot (b-a) \tag{6}$$

Figure 4: The Midpoint Rule for Approximating a Definite Integral

Approximating the solution to example 1.1 using the midpoint rule yields:

$$\begin{aligned}
I &= \int_1^{1.2} \frac{1}{t}\mathrm{dt} \\
&\approx I_M \\
&= f(1.1) \cdot (1.2 - 1) \\
&= \frac{1}{1.1} \cdot 0.2 \\
&= 0.1818\ldots
\end{aligned}$$

We can summarize the midpoint rule by the notation

$$\left\{ \frac{a+b}{2} \right\}$$

This notation means that the midpoint rule approximates the integral $\int_a^b f(t)\,dt$ by evaluating f at $\frac{a+b}{2}$, finding the polynomial which interpolates this point, and integrating this polynomial.

2.3 Trapezoid Rule

In the *trapezoid rule*, we approximate $f|_{[a,b]}$ using the endpoints of the interval $[a,b]$ as our interpolation. The polynomial interpolant will thus be a linear polynomial (with degree at most 1) passing through $f(a)$ and $f(b)$, as shown in Figure 5 and we can calculate its area I_T simply, using

$$\begin{aligned}
I_T &= \frac{f(a) + f(b)}{2} \cdot (b - a) & (7) \\
&= \frac{1}{2} f(a) \cdot (b - a) + \frac{1}{2} f(b) \cdot (b - a) & (8)
\end{aligned}$$

Note that the two weights w_0, w_1 in this case are each $1/2 \cdot (b - a)$. The sum of the weights will *always* equal the width of the interval $(b - a)$.
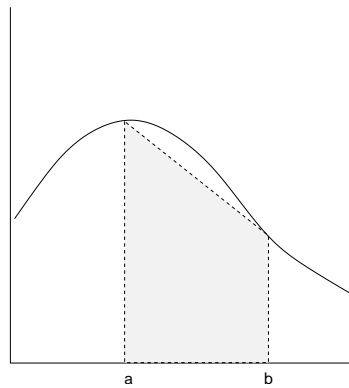

Figure 5: The Trapezoid Rule for Approximating a Definite Integral

Approximating the solution to example 1.1 using the trapezoid rule yields:

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$$\begin{aligned} I &= \int_1^{1.2} \frac{1}{t}\mathrm{dt} \\ &\approx I_T \\ &= \frac{f(1) + f(1.2)}{2} \cdot (1.2 - 1) \\ &= \frac{1}{2} \cdot \left(\frac{1}{1} + \frac{1}{1.2}\right) \cdot 0.2 \\ &= 0.183333\ldots \end{aligned}$$

We can summarize the trapezoid rule by the notation

$$\{a, b\}$$

This notation means that the trapezoid rule approximates the integral $\int_a^b f(t)\,dt$ by evaluating f at a and b, finding the polynomial which interpolates these two points, and integrating this polynomial.

2.4 Simpson's Rule

In *Simpson's rule*, we approximate $f|_{[a,b]}$ using three equidistant interpolation points $[a, \frac{a+b}{2}, b]$, corresponding to the endpoints and midpoint of the interval. The resulting polynomial interpolant will thus have degree at most 2, as shown in Figure 6 and can be written as:

$$p(t) = f(a) \cdot \frac{(t-m)(t-b)}{(a-m)(a-b)} + f(m) \cdot \frac{(t-a)(t-b)}{(m-a)(m-b)} + f(b) \cdot \frac{(t-m)(t-a)}{(b-m)(b-a)}$$

where m is the midpoint $\frac{a+b}{2}$. Integrating the Lagrange polynomials over $[a, b]$ gives the following formula for the area I_S:

$$I_S = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] \tag{9}$$

note again that the weights $\frac{b-a}{6}$, $4 \cdot \frac{b-a}{6}$, $\frac{b-a}{6}$ add up to the width of the interval $(b-a)$.

Approximating the solution to example 1.1 using Simpson's rule yields:

$$\begin{aligned} I &= \int_1^{1.2} \frac{1}{t}\mathrm{dt} \\ &\approx I_S \\ &= \frac{1.2 - 1}{6}\left[f(1) + 4 \cdot f(1.1) + f(1.2)\right] \\ &= \frac{0.2}{6}\left[\frac{1}{1} + \frac{4}{1.1} + \frac{1}{1.2}\right] \\ &= 0.182323\ldots \end{aligned}$$

We can summarize Simpson's rule by the notation

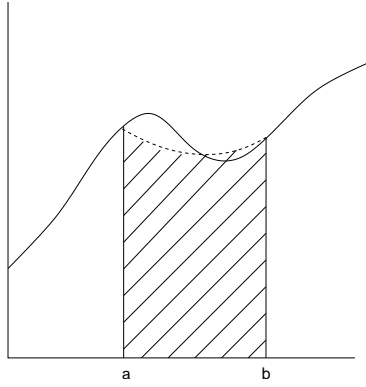$$\left\{a, \frac{a+b}{2}, b\right\}$$

Figure 6: Simpson's Rule for Approximating a Definite Integral

This notation means that Simpson's rule approximates the integral $\int_a^b f(t)\,dt$ by evaluating f at a, $\frac{a+b}{2}$, and b, finding the polynomial which interpolates these three points, and integrating this polynomial.

3   Error Analysis

Since we used polynomial interpolation as the basis for each of the basic rules for approximating the definite integral, we can use the error formula for polynomial interpolation to calculate the error. For any of these rules, we can calculate the error E_{rule} as:

$$
\begin{aligned}
E_{\text{rule}} &= I - I_{\text{rule}} \\
&= \int_a^b f(t)\mathrm{dt} - \int_a^b p(t)\mathrm{dt} \\
&= \int_a^b [f(t) - p(t)]\,\mathrm{dt}
\end{aligned}
$$

We can use the error formula for polynomial interpolation over $n+1$ points to express $f(t)-p(t)$

$$
f(t) - p(t) = \frac{f^{n+1}(c)}{(n+1)!}(t - x_0)(t - x_1)\dots(t - x_n)
$$

where c is a point that exists *somewhere* on the interval. It is important to note that this is not an approximation of the error, but an *exact* error formula. Substituting into the error formula for approximating definite integrals yields:

$$
\begin{aligned}
E_{\text{rule}} &= \int_a^b \frac{f^{n+1}(c)}{(n+1)!}(t - x_0)(t - x_1)\dots(t - x_n)\mathrm{dt} \\
&= \frac{f^{n+1}(c)}{(n+1)!} \cdot \int_a^b \underbrace{(t - x_0)(t - x_1)\dots(t - x_n)}_{\omega(t)}
\end{aligned}
$$

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We cannot calculate this error exactly (since we don't know c), but we will consider two cases for $\omega(t)$. These cases are not *exhaustive*, but they do cover all four simple rules (and, in fact, all interesting rules of this kind).

Case 1

$\omega(t)$ does not change sign on $[a, b]$. That is, either

$$\omega|_{[a,b]} \geq 0 \quad \text{or}$$
$$\omega|_{[a,b]} \leq 0$$

Case 2

$$\int_a^b \omega(t)\mathrm{dt} = 0$$

3.1   Case 1

Which of the rules have $\omega(t)$ not changing sign over $[a, b]$?

Rectangle Rule

For the rectangle rule, $\omega(t) = t - a$, which is always positive on the interval, so the rectangle rule falls into case 1.

Midpoint Rule

For the midpoint rule, $\omega(t) = t - (a + b)/2$, which is negative to the left of the midpoint and positive to the right of the midpoint, so the midpoint rule does not fall into case 1.

Trapezoid Rule

For the trapezoid rule, $\omega(t) = (t - a)(t - b)$. On (a, b), this value is always negative, since $t - a$ is always positive and $t - b$ is always negative. Thus, the trapezoid rule falls into case 1.

Simpson's Rule

In Simpson's rule, $\omega(t) = (t - a)[t - (a + b)/2](t - b)$. Since $(t - a)(t - b)$ is always negative, and $t - (a + b)/2$ flips signs on either side of the midpoint, Simpson's rule does not fall into case 1.

3.1.1   Error Analysis of Rectangle Rule

For rules that match case 1, we have

$$E_{\text{rule}} \;=\; \frac{f^{(n+1)}(c)}{(n + 1)!} \int_a^b \omega(t)\mathrm{dt}$$

for the rectangle rule, this becomes:

$$
\begin{aligned}
E_R &= f'(c) \int_a^b (t - a)\mathrm{dt} \\
&= \frac{f'(c)}{2} \cdot (b - a)^2
\end{aligned}
$$

Note that the width of the interval $(b - a)$ is raised to the second power in this error. As we will see in later lectures, we would like this power to be as large as possible, so that the error will shrink rapidly as the width of the interval decreases.

It is important to note that the errors we obtain using this method are exact error expressions. A negative error (which will depend both on the sign of the error expression and the sign of the function's derivative) indicates that the method is overestimating the error, so that we could adjust our estimate using the error expression. Looking at example 1.1 we see that our error is given by:

$$
\begin{aligned}
E_R &= \frac{f'(c)}{2} \cdot (b - a)^2 \\
&= -\frac{1}{2 \cdot c^2} \cdot (0.2)^2 \\
&= -\frac{0.02}{c^2}
\end{aligned}
$$

This indicates that our approximation that $I \cong 0.2$ was an overestimate by at most 0.02.

3.1.2   Error Analysis of Trapezoid Rule

For the trapezoid rule, we have error:

$$
\begin{aligned}
E_T &= \frac{f''(c)}{2} \int_a^b (t - a)(t - b)\mathrm{dt} \\
&= \frac{f''(c)}{2} \left(-\frac{(b - a)^3}{6} \right) \\
&= -\frac{f''(c)}{12} (b - a)^3
\end{aligned}
$$

Looking at example 1.1 we see that our error is given by:

$$
\begin{aligned}
E_T &= -\frac{f''(c)}{12} (b - a)^3 \\
&= -\frac{1}{6 \cdot c^3} \cdot (0.2)^3 \\
&= -\frac{0.01333\ldots}{c^3}
\end{aligned}
$$

This indicates that our approximation that $I \cong 0.18333\ldots$ was an overestimate by at most 0.0133.

3.2 Case 2

Case 2 demands that

$$\int_a^b \omega(t)\mathrm{dt} \;=\; 0 \tag{10}$$

It is easy to see that this condition holds for both the midpoint rule and Simpson's rule. An interesting feature of rules that match case 2 is that adding a point to the polynomial interpolation results in no difference in the estimate of the area of the interpolant over $[a, b]$. We know this is true, since equation 10 tells us that the definite integral of the next Newton polynomial over $[a, b]$ is zero. This means that we can calculate the error for any rule matching case 2 by adding an additional point to the interpolation. We will discuss this in the next lecture.