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1 Integration

1.1 Motivation

Recall the limit definition of a definite Riemann integral:
Let \([a, b]\) be a closed interval on the real line and a partition of \([a, b]\) be a finite sequence \(t_1, t_2, \ldots, t_n\) such that

\[
a = x_0 \leq t_1 \leq x_1 \leq t_2 \leq x_2 \leq \cdots \leq x_{n-1} \leq t_n \leq x_n = b
\]

and for convenience we take an equispaced partition so that \(h = \frac{b-a}{n}\). Then a Riemann sum of a function with respect to this partition is given by

\[
\int_a^b f(x) \, dx = \lim_{n \to \infty} \left( \frac{b - a}{n} \right) \sum_{i=1}^{n} f(t_i)
\]

What is this really saying? It says that we break up our domain into a bunch of equispaced pieces (of length \(\frac{b-a}{n}\)) and attempt to approximate the integral on each piece by a single rectangle. As the number of pieces goes to infinity (or equivalently the size of each piece goes to zero), our approximation approaches the true integral in the limit. This is how all of our numerical integration schemes are motivated: break up the domain into finitely many pieces, and attempt to approximate the integral on each piece.

We need numerical integration because most of the time, our usual notion of definite integration via the fundamental theorem of calculus and antiderivatives fail, for the simple reason that most elementary functions do not have antiderivatives, yet certainly the value of this integral (interpreted as area under the curve) certainly still exists and we want to find it.

1.2 Basic Quadrature Rules

Let’s start off with the simplifying assumption that we don’t break up the domain at all and try to evaluate the integral on the whole interval \([a, b]\). The idea is that we will replace \(f(x)\) with interpolating polynomials \(P(x)\) of higher and higher degree, and since polynomials are easy to integrate, use the result as an approximation.

The simplest thing we could do is replace our function with a degree 0 polynomial (a horizontal line). All we need to do is pick a single point to interpolate \(P_0\) through. We could either pick the left endpoint, the right endpoint, or the midpoint.

The next thing we could do is interpolate a degree 1 polynomial. The natural choice is to pick both the endpoints, and this is the Trapezoid rule.
We could go further and pick a degree 2 polynomial fit through three equispaced points (left endpoint, midpoint, and right endpoint) and this would be Simpson’s rule.

Now the natural question is, how good are these approximations? Since we have an expression for error in polynomial interpolation:

\[ f(x) = P(x) + \frac{f^{(n+1)}(\xi)}{(n+1)!} (x - x_0)(x - x_1) \cdots (x - x_n) \quad \xi \in (x_0, x_n) \]

We can simply integrate this expression from \(a\) to \(b\) w.r.t \(x\) to get an error for these integrals we approximate by replacing \(f\) with an interpolant:

\[ \int_a^b f(x) \, dx = \int_a^b P(x) \, dx + \int_a^b \frac{f^{(n+1)}(\xi)}{(n+1)!} (x - x_0)(x - x_1) \cdots (x - x_n) \, dx \quad \xi \in (x_0, x_n) \]

Let’s do this for the Trapezoid Rule (note \(x_0 = a, x_1 = b\)).

\[ f(x) = \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1) + \frac{1}{2} \frac{f''(\xi)(x - x_0)(x - x_1)}{R(x)} \]
Let’s compute the integral of \( P(x) \) to get the Quadrature rule:

\[
\int_a^b P(x) \, dx = \int_a^b \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1) \, dx \\
= \left[ \frac{(x - x_1)^2}{2(x_0 - x_1)} f(x_0) + \frac{(x - x_0)^2}{2(x_1 - x_0)} f(x_1) \right]_{x_0}^{x_1} \\
= \frac{(x_1 - x_0)}{2} [f(x_0) + f(x_1)] \\
= \frac{h}{2} (f(a) + f(b))
\]

Now let’s integrate the error term from interpolation to get the error term for quadrature:

\[
\int_a^b R(x) \, dx = \frac{1}{2} f''(\xi) \int_a^b (x - x_0)(x - x_1) \, dx \\
= \frac{1}{2} f''(\xi) \int_a^b (x^2 - (x_0 + x_1)x + x_0x_1) \, dx \\
= \frac{1}{2} f''(\xi) \left[ \frac{x^3}{3} - \frac{(x_1 + x_0)x^2}{2} - x_0x_1x \right]_{x_0}^{x_1} \\
= -\frac{h^3}{12} f''(\xi)
\]

So the Trapezoid Rule is given by

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

You can follow an analogous procedure to get Simpson’s Rule:

\[
\int_a^b f(x) \, dx = \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90} f^{(4)}(\xi)
\]

### 1.3 Composite Quadrature Rules

The idea behind a composite quadrature rule is as follows: instead of trying to replace \( f \) on the entire interval of integration by an interpolant, break up the domain into equispaced pieces, and then on each small piece, approximate by an interpolant. The motivation for this is very similar to the one for Cubic Splines.

So here is how you can turn a integration rule and error term on the whole interval into a composite one. Recall Simpson’s rule for the interval interval is given by:

\[
\int_a^b f(x) \, dx \approx \frac{h}{3} \left[ f(a) + 4f \left( \frac{a + b}{2} \right) + f(b) \right]
\]
We got this by replacing the integrand with the interpolant at three points, left endpoint, midpoint, and right endpoint. The error bound for interpolation gives us:

\[
\int_{a}^{b} f(x) \, dx = \frac{h}{3} \left[ f(a) + 4f \left( \frac{a+b}{2} \right) + f(b) \right] - \frac{h^5}{90} f^{(4)}(\xi) \quad \xi \in (a, b)
\]

Let’s derive the composite rule by dividing the domain into \( n \) equally spaced intervals and apply the quadrature rule on each consecutive pair of subintervals (because of this \( n \) must be even).

With \( h = \frac{b-a}{n} \) and \( x_j = a + jh, j = 0, 1, \ldots, n \), we have that:

\[
\int_{a}^{b} f(x) \, dx = \int_{x_0}^{x_2} f(x) \, dx + \int_{x_2}^{x_4} f(x) \, dx + \cdots + \int_{x_{n-2}}^{x_n} f(x) \, dx
\]

\[
= \sum_{j=1}^{n/2} \int_{x_{2j-2}}^{x_{2j}} f(x) \, dx
\]

\[
= \sum_{j=1}^{n/2} \left( \frac{h}{3} [f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j})] - \frac{h^5}{90} f^{(4)}(\xi_j) \right) \quad \xi_j \in (x_{2j-2}, x_{2j})
\]

\[
= \frac{h}{3} \left[ f(x_0) + 2 \sum_{j=1}^{n/2-1} f(x_{2j}) + 4 \sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n) \right] - \frac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi_j)
\]

That big thing in the square brackets is just saying that an error rule with coefficients \([1, 4, 1]\) becomes a composite rule with coefficients \([1, 4, 2, 4, 2, 4, \ldots, 2, 4, 2, 4, 1]\).

Now we see that the error form of the composite rule is given by

\[
E(f) = -\frac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi_j) \quad \xi_j \in (x_{2j-2}, x_{2j})
\]
We know by the extreme value theorem that
\[
\min_{x \in [a,b]} f^{(4)}(x) \leq f^{(4)}(\xi_j) \leq \max_{x \in [a,b]} f^{(4)}(x)
\]
\[
\frac{n}{2} \min_{x \in [a,b]} f^{(4)}(x) \leq \sum_{j=1}^{n/2} f^{(4)}(\xi_j) \leq \frac{n}{2} \max_{x \in [a,b]} f^{(4)}(x)
\]
\[
\min_{x \in [a,b]} f^{(4)}(x) \leq \frac{2}{n} \sum_{j=1}^{n/2} f^{(4)}(\xi_j) \leq \max_{x \in [a,b]} f^{(4)}(x)
\]

By the Intermediate Value Theorem applied on \( f^{(4)} \), there exists \( \mu \in (a,b) \) such that
\[
f^{(4)}(\mu) = \frac{2}{n} \sum_{j=1}^{n/2} f^{(4)}(\xi_j)
\]

So this implies the error of the composite rule is given by:
\[
E(f) = -\frac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi_j) = -\frac{h^5}{180} n f^{(4)}(\mu) = -\frac{(b-a)}{180} h^4 f^{(4)}(\mu)
\]

For another example, see one of Ming’s old exam questions. He gives you a quadrature rule called Boole’s rule and you can construct and apply that as a composite rule. Here is a computational example using Composite Simpson’s rule.

**Example 1** Use the \( n = 6 \) Simpson’s rule to evaluate \( \int_0^\pi \sin(x) \, dx \). Then compute a bound on the error using \( E = -\frac{b-a}{180} h^4 f^{(4)}(\xi) \).

**Solution:** Since \( a = 0, b = \pi \), we have that \( h = \frac{b-a}{n} = \frac{\pi}{6} \). So our integral estimate \( S(h) \) is given by

\[
S(h) = \frac{h}{3} \begin{bmatrix} f(x_0) \\ f(x_1) \\ \vdots \\ f(x_6) \end{bmatrix} = \frac{\pi}{18} \left( 0 + 4 \left( \frac{1}{2} \right) + 2 \left( \frac{\sqrt{3}}{2} \right) + 4(1) + 2 \left( \frac{\sqrt{3}}{2} \right) + 4 \left( \frac{1}{2} \right) + 0 \right)
\]
\[
= \frac{\pi}{18} \left( 2 + \sqrt{3} + 4 + 2\sqrt{3} + 2 \right) = \frac{\pi}{18} (8 + 2\sqrt{3}) = \frac{\pi}{9} (4 + \sqrt{3})
\]

As for the error estimate, since \( f(x) = \sin(x) \), we also have \( f^{(4)}(x) = \sin(x) \). This gives us that
\[
|E| = \left| -\frac{\pi}{180} \left( \frac{\pi}{6} \right)^4 \sin(\xi) \right| \leq \frac{\pi^5}{180(6^4)}
\]

**Comment:** The other kind of question that gets asked with these error bounds is to find a minimum \( n \) (or equivalently a maximum \( h \)), such that an approximation with a given scheme will result in an error less than some given tolerance \( \epsilon \).
1.4 Degree of Precision

The **degree of precision** (or accuracy) of a quadrature formula is the largest positive integer \( n \) such that the formula holds exactly for \( x^k \) for all \( k = 0, 1, \ldots n \). This is by far the most common type of question so we will do lots of examples.

In all the previous cases, we can tell the degree of precision by the construction of the rule. Recall we replace the function with an interpolating polynomial and integrate. The degree of precision is exactly the degree of the interpolant. For example, the trapezoid rule has degree of precision 1, and Simpson’s rule has degree of precision 2.

**Question:** If we take a quadrature rule and extend it to a composite quadrature rule, does its degree of precision change?

**Example 2** Find the degree of precision of the quadrature formula:

\[
\int_{-1}^{1} f(x) \, dx = f \left( -\frac{\sqrt{3}}{3} \right) + f \left( \frac{\sqrt{3}}{3} \right)
\]

**Solution:** Let’s start testing monomials of increasing powers:

- \( f = 1 \Rightarrow 2 = 1 + 1 \, \checkmark \)
- \( f = x \Rightarrow 0 = -\frac{\sqrt{3}}{3} + \frac{\sqrt{3}}{3} \, \checkmark \)
- \( f = x^2 \Rightarrow \frac{2}{3} = \frac{1}{3} + \frac{1}{3} \, \checkmark \)
- \( f = x^3 \Rightarrow 0 = -\frac{1}{3\sqrt{3}} + \frac{1}{3\sqrt{3}} \, \checkmark \)
- \( f = x^4 \Rightarrow 2 \frac{5}{9} = \frac{1}{9} + \frac{1}{9} \, \times \)

So by definition, this quadrature rule has degree of precision 3.

**Comment 1:** Note all the integrals of the monomials of odd powers are automatically zero, because the integral of an odd function over a symmetric function is zero.

**Comment 2:** This implies that this quadrature rule is exact for all cubics, since every cubic is just a linear combination of \( \{1, x, x^2, x^3\} \).

**Comment 3:** Don’t forgot to check it holds for \( f = 1 \) first! (I don’t know why students always seem to ignore this). Just because a quadrature rule holds for a higher power (or powers) does not mean it automatically holds for all lower powers. For example, this quadrature rule is true for all monomials of odd power (in particular \( x^5 \)), but as we can see its certainly not true for \( x^4 \).
Example 3  Given a quadrature rule of the form:

$$\int_{-1}^{1} f(x) \, dx = c_0 f(-1) + c_1 f(0) + c_2 f(1)$$

Find constants $c_0, c_1, c_2$ so that this rule has as high a degree of precision as possible. What is the resulting degree of precision?

Solution: We want this rule to be exact for as many monomial powers as possible starting with $f = 1$. So enforcing that gives us:

Exact for $f = 1$: $\implies 2 = c_0 + c_1 + c_2$

We might expect that since we have three constants, we can enforce three conditions, so:

Exact for $f = x$: $\implies 0 = -c_0 + c_2$

Exact for $f = x^2$: $\implies \frac{2}{3} = c_0 + c_2$

Solving this simple $3 \times 3$ system gives us $c_0 = \frac{1}{3}, c_1 = \frac{4}{3}, c_2 = \frac{1}{3}$, so our quadrature rule is

$$\int_{-1}^{1} f(x) \, dx = \frac{1}{3} f(-1) + \frac{4}{3} f(0) + \frac{1}{3} f(1)$$

By design this has degree of precision AT LEAST 2, let’s just check it for cubics:

$$f = x^3 \implies 0 = -\frac{1}{3} + \frac{1}{3} \checkmark$$

So by magic it does hold for $f = x^3$ even though we didn’t design it that way. (The magic here is really symmetric). Now let’s check $f = x^4$:

$$f = x^4 \implies \frac{2}{5} = \frac{1}{3} + \frac{1}{3} \times$$

and the magic has run out. So the degree of precision of the quadrature rule is 3.

These are the two basic types of problem. Let’s do some variations on the latter.

Example 4 Let $w(x) = \sqrt{x}$. Find a numerical integration scheme

$$\int_{0}^{1} w(x) f(x) \, dx \approx c_0 f(0) + c_1 f(x_1)$$

that is exact for polynomials $f(x)$ of degree $\leq 2$. 
Solution: This is very similar to the last problem, except it now its a “weighted integral” (with weight function $w(x)$). But nothing changes in how we approach this. We must find the three constants such that this rule is exact for $f = 1, x, x^2$.

Since we want to test this rule for $f(x) = x^k, k = 0, 1, 2$, the LHS always has the form:

$$\int_0^1 x^{k+\frac{1}{2}} \, dx = \left. \frac{1}{k + 3/2} x^{k+\frac{3}{2}} \right|_0^1 = \frac{2}{2k + 3}$$

Exact for $f = 1$: $\Rightarrow \frac{2}{3} = c_0 + c_1$

Exact for $f = x$: $\Rightarrow \frac{2}{5} = c_1 x_1$

Exact for $f = x^2$: $\Rightarrow \frac{2}{7} = c_1 x_1^2$

Solving this system gives us $c_0 = \frac{8}{75}, c_1 = \frac{14}{25}, x_1 = \frac{5}{7}$.

Example 5 Let $p \in (-1, \infty)$ and $w(x) = x^p$. Find a numerical integration scheme

$$\int_0^1 w(x)f(x) \, dx \approx c_0 f(0) + c_1 f(x_1)$$

that is exact for polynomials $f(x)$ of degree $\leq 2$.

Solution: This problem is a slight generalization to the previous one but the weight function seems to trip people up a bit.

Since we want to test this rule for $f(x) = x^k, k = 0, 1, 2$, the LHS always has the form:

$$\int_0^1 x^{k+p} \, dx = \left. \frac{x^{k+p+1}}{k+p+1} \right|_0^1 = \frac{1}{k+p+1}$$

Exact for $f = 1$: $\Rightarrow \frac{1}{p+1} = c_0 + c_1$

Exact for $f = x$: $\Rightarrow \frac{1}{p+2} = c_1 x_1$

Exact for $f = x^2$: $\Rightarrow \frac{1}{p+3} = c_1 x_1^2$

$x_1$ is the easiest to solve for first, and you get $x_1 = \frac{p+2}{p+3}$. Then solve for $c_1 = \frac{1}{x_1(p+2)} = \frac{p+3}{(p+2)^2}$. Then finally $c_0 = \frac{1}{p+1} - c_1 = \frac{1}{p+1} - \frac{(p+3)}{(p+2)^2}$. It is nice to check this reduces to the result in the previous question for $p = \frac{1}{2}$.
Example 6 Determine the constants $a, b, \alpha$ such that the quadrature rule
\[ \int_{-1}^{1} f(x) \, dx \approx af(-1) + af(1) + bf(\alpha) + bf(-\alpha) \]
has the highest possible degree of precision. Clearly state the degree of precision of the resulting rule. Then use the quadrature rule to approximate the integral below. Use $a, b, \alpha$ instead of the values calculated in the previous part.

\[ \int_{0}^{4} e^{\sqrt{x}} \, dx \]

Solution: We need to evaluate the quadrature rule for compare the LHS and RHS for monomials $f(x) = x^k$:

\[
\begin{align*}
\text{n odd} &= \left\{ \begin{array}{l}
\int_{-1}^{1} x^k \, dx = 0 \\
af(-1) + af(1) + bf(\alpha) + bf(-\alpha) = 0
\end{array} \right.
\end{align*}
\]
\[
\begin{align*}
\text{n even} &= \left\{ \begin{array}{l}
\int_{-1}^{1} x^k \, dx = \frac{2^{k+1}}{k+1} \\
af(-1) + af(1) + bf(\alpha) + bf(-\alpha) = 2a + 2b\alpha^k
\end{array} \right.
\end{align*}
\]
So it’s clear that the monomials with odd powers give us no information, since the quadrature rule is valid for any choice of $a, b, \alpha$. So let’s look at $k = 0, 2, 4$ and solve for $a, b, \alpha$:

\[
\begin{align*}
\begin{cases}
2a + 2b = 2 \\
2a + 2b\alpha^2 = \frac{2}{3} \\
2a + 2b\alpha^4 = \frac{2}{5}
\end{cases} \quad \Rightarrow \quad \begin{cases}
2b(1 - \alpha^2) = \frac{4}{3} \\
2b(1 - \alpha^4) = \frac{8}{5}
\end{cases} \quad \Rightarrow \quad \frac{1 - \alpha^2}{1 - \alpha^4} = \frac{5}{6}
\end{align*}
\]

\[
5\alpha^4 - 6\alpha^2 + 1 = 0 \quad \Rightarrow \quad \alpha^2 = \frac{3}{5} \pm \sqrt{\frac{9}{25} - \frac{1}{5}} = \frac{3}{5} \pm \frac{2}{5} = \frac{1}{5}, 1
\]
The solution $\alpha^2 = 1$ is clearly invalid, so we pick the positive root $\alpha = \frac{1}{5}$. The weights are then $a = \frac{1}{6}, b = \frac{5}{6}$, and then the degree of precision of the resulting rule is 5.

We cannot directly apply the quadrature rule to the integral in the current form because the integral is from $[0, 4]$ and the quadrature rule only applies to integrals on $[-1, 1]$. So do a simple change of variables from Math 1A. The change of variables that will transform $x \in [0, 4]$ to $u \in [-1, 1]$ is given by $u = x/2 - 1 \quad \Rightarrow \quad x = 2u + 2, \, dx = 2du$.

\[
\int_{0}^{4} e^{\sqrt{x}} \, dx = 2 \int_{-1}^{1} e^{\sqrt{2+2u}} \, du \approx 2(ae^0 + ae^{\sqrt{2}} + be^{\sqrt{2+2\alpha}} + be^{\sqrt{2-2\alpha}})
\]