Chapter 3

Integrals and Limits

3.1 Origins of the concept of integration

We begin with the early work by the pioneers Archimedes and Cavalieri who showed how to integrate x^2 and x^k respectively. In modern formulas, we want to show how to integrate $\int_0^1 x^k$. The strategy is to relate these integrals to sums of powers of integers. We start by taking the interval of 0 to 1 and divide into n intervals running from $\frac{0}{n}$ to $\frac{n}{n}$.

The red rectangles have an area less than the integral, while the green rectangles cover a larger area. This sounds like we will be invoking the "squeeze principle" again. Indeed, we will. Let t_n denote the sum of the green rectangles and s_n the sum of the blue rectangles.

$$t_n = \left(\frac{1}{n}\right)^k \cdot \frac{1}{n} + \left(\frac{2}{n}\right)^k \cdot \frac{1}{n} + \left(\frac{3}{n}\right)^k \cdot \frac{1}{n} + ... + \left(\frac{n}{n}\right)^k \cdot \frac{1}{n} \tag{3.1}$$

$$s_n = \left(\frac{0}{n}\right)^k \cdot \frac{1}{n} + \left(\frac{1}{n}\right)^k \cdot \frac{1}{n} + \left(\frac{2}{n}\right)^k \cdot \frac{1}{n} + ... + \left(\frac{n-1}{n}\right)^k \cdot \frac{1}{n} \tag{3.2}$$

So

$$s_n \leq \int_0^1 x^k \leq t_n \tag{3.3}$$

But

$$t_n = \sum_{j=1}^{n} \frac{j^k}{n^{k+1}}, \tag{3.4}$$

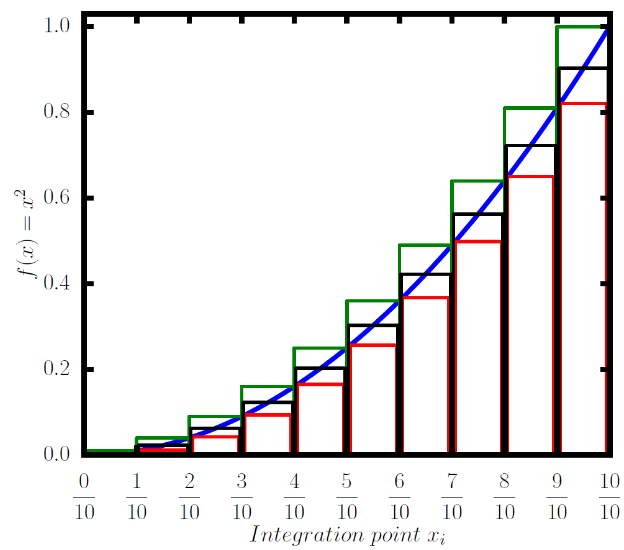

Figure 3.1: Three different rectangular integration routines for $\int_0^1 x^k\,dx$ with $k=2$. The function is plotted in blue, the three different numerical integration schemes are left point (red), midpoint (black) and right point (green). One can clearly see the integral is bounded to lie in between the sum of the red and green rectangular areas.

and

$$s_n = \sum_{j=0}^{n-1} \frac{j^k}{n^{k+1}} = \sum_{j=1}^{n-1} \frac{j^k}{n^{k+1}}, \tag{3.5}$$

where in the second equality in the s_n equation, we note that we can drop the $j=0$ term.

Now we invoke the critical piece of the squeeze argument. To begin, note that $t_n - s_n = \frac{1}{n}$ so as $n \to \infty$, $t_n - s_n \to 0$ or $t_n \to s_n$ and this limit is the integral. How do we know this result, that $t_n - s_n = \frac{1}{n}$? Each term in s_n also appears in t_n. But t_n has one more term—its last term. Hence, the difference is precisely that last term $\frac{n^k}{n^{k+1}} = \frac{1}{n}$. Then the rest of the argument follows as above. To determine the final result, we need to now evaluate these finite sums of powers of integers.

3.2 Sums of powers of integers

The skill to learn how to sum powers of integers is a useful one. You might think it is an odd thing to do, as we cannot extend these sums to infinity (unlike some popular youtube videos would say), because such sums always *diverge*. But we can actually get closed-form expressions for *finite summations*. And this is a rather marvelous result. We show you how to do this next.

Define

$$\mathrm{sum}_k(n) = \sum_{j=1}^{n} j^k = \text{ sum of first n integers raised to the k power.} \tag{3.6}$$

The simplest case is $k = 1$.

$$\mathrm{sum}_1(n) = 1 + 2 + 3 + ... + n. \tag{3.7}$$

We can write $\mathrm{sum}_1(n)$ in reverse order underneath, and add down the columns:

$$\begin{aligned} \mathrm{sum}_1(n) &= 1 + \quad 2 \quad + \quad 3 \quad + \ldots + n \\ \mathrm{sum}_1(n) &= n + (n-1) + (n-2) + \ldots + 1 \end{aligned} \tag{3.8}$$

$$2 \times \mathrm{sum}_1(n) = \underbrace{(n+1) + (n+1) + (n+1) + ... + (n+1)}_{n \text{ terms}} \tag{3.9}$$

There are n terms of $(n + 1)$, so

$$\mathrm{sum}_1(n) = \frac{n(n+1)}{2}. \tag{3.10}$$

This result is very direct, simple and neat.

Unfortunately, this approach is not easily generalized to other k powers. So we have to proceed a different way. We do so by computing differences of finite sums in two different ways. Consider

$$\sum_{j=1}^{n} \left[(j+1)^2 - j^2\right] = (n+1)^2 - 1 = n^2 + 2n, \tag{3.11}$$

which follows since many of the terms (all except the first term of the second sum and the last term of the first sum) cancel when the sums are subtracted from ach other. Now, we compute a second way, by expanding the terms in the sums (this is mathematically fine because all sums are *finite*). We find

$$\sum_{j=1}^{n}\left[(j+1)^2-j^2\right]=\sum_{j=1}^{n}\left(\cancel{j^2}+2j+1-\cancel{j^2}\right)=\sum_{j=1}^{n}2j+\sum_{j=1}^{n}1 \tag{3.12}$$

We realize that

$$\sum_{j=1}^{n}2j=2\sum_{j=1}^{n}1 \tag{3.13}$$

and

$$\sum_{j=1}^{n}1=n. \tag{3.14}$$

So we immediately discover (after equating the two ways to evaluate the summations) that

$$2\,\mathrm{sum}_1(n)=n^2+2n-n=n(n+1) \tag{3.15}$$

so

$$\mathrm{sum}_1(n)=\frac{n(n+1)}{2} \tag{3.16}$$

as before.

But this strategy can be generalized to higher powers of k.

We can check the next case where we work with cubes instead of squares. We have

$$\sum_{j=1}^{n}\left[(j+1)^3-j^3\right]=(n+1)^3-1=n^3+3n^2+3n \tag{3.17}$$

and

$$\begin{aligned}\sum_{j=1}^{n}\left[(j+1)^3-j^3\right]&=\sum_{j=1}^{n}\left(\cancel{j^3}+3j^2+3j+1-\cancel{j^3}\right) &(3.18)\\ &=3\,\mathrm{sum}_2(n)+3\,\mathrm{sum}_1(n)+\mathrm{sum}_0(n) &(3.19)\\ &=n^3+3n^2+3n. &(3.20)\end{aligned}$$

So

$$\mathrm{sum}_2(n) = \frac{1}{3}\left(\underbrace{n^3+3n^2+3n}_{\text{sum first way}}\underbrace{-\frac{3}{2}n^2-\frac{3}{2}n}_{-3\,\mathrm{sum}_1(n)}\underbrace{-n}_{-\mathrm{sum}_0(n)}\right) \tag{3.21}$$

$$= \frac{1}{3}\left(n^3+n^2+\frac{1}{2}n\right) \tag{3.22}$$

$$= \frac{1}{6}n\left(2n^2+3n+1\right) \tag{3.23}$$

$$= \frac{1}{6}n\left(2n+1\right)\left(n+1\right). \tag{3.24}$$

Hence, we have found that

$$\sum_{j=1}^{n} j^2 = \frac{1}{6}n(2n+1)(n+1). \tag{3.25}$$

For the $k=2$ case, the integral of the parabola then gives

$$\int_0^1 x^2\,dx = \lim_{n\to\infty}\frac{1}{6}n(2n+1)(n+1)\frac{1}{n^3} = \frac{1}{3} \tag{3.26}$$

as expected. One can use this technique to calculate higher integer powers as well. Cavalieri extended this to all the way to $k=10$. The strategy is to extend the expression for the difference of the sums of powers to higher k values. The highest-order terms, proportional to j^k cancel in the two summations. Then the procedure continues as we did above. We need to use the results for all previous powers to obtain the final answer. Note that there does not seem to be any simply pattern to these final answers, so we do not try to establish them by induction. But if you like, you could determine the result for the highest power of n (proportional to n^{k+1}), which is what is needed for the calculation of the integral.

Fermat used a slightly different method, with an infinite number of steps and the identity

$$\lim_{x\to 1}\frac{1-x^{k+1}}{1-x} = \lim_{x\to 1}\left(1+x+x^2+x^3+...+x^k\right) = k+1 \tag{3.27}$$

to prove the integral result for all integer k.

3.3 Issues with defining an integral

The book discusses issues with defining an integral in greater depth, but the main results are

- The integral is well defined for piecewise monotonic (strictly increasing or decreasing) functions
- Strange functions (like the one in section 17) show that one has to be careful and precise in defining the integral. This often does not play a role in integrals that arise in physics, but occasionally is relevant in some areas like Cantor sets or strange attractors. The field of real analysis spends significant time sorting out all possible subtleties in how one defines an integral.
- *The definite integral is not the area under the curve.* It is often that one can think of it as the *signed* area under the curve, where negative values correspond to negative areas.

3.4 Numerical integration

We do not go into detail into numerical techniques in this class, but it is important for you to know some of the basics. Below is a crash course on numerical quadrature.

While the definite integral is defined in the limit where the maximal step size approaches 0, we must work with a finite step size to calculate a numerical approximation to the integral. The simplest quadrature rule is a left point, midpoint, or right point integration rule. These are demonstrated in Fig. 3.2.

We call the coordinate where the function is evaluated x_i, and the value of the function used $f(x_i)$. Then the numerical approximation to the integral replaces the integral with a finite sum of terms

$$\int_a^b f(x)\,dx = \Delta x \sum_{i=1}^{n} f(x_i) \tag{3.28}$$

where the $\{x_i\}$ are chosen as described in Fig. 3.2, corresponding to the specific integration rule that is being used. For example, in left-point integration, we choose $\Delta x = (b-a)/n$ and $x_i^{\text{left}} = (i-1)\Delta x$. The right point rule is

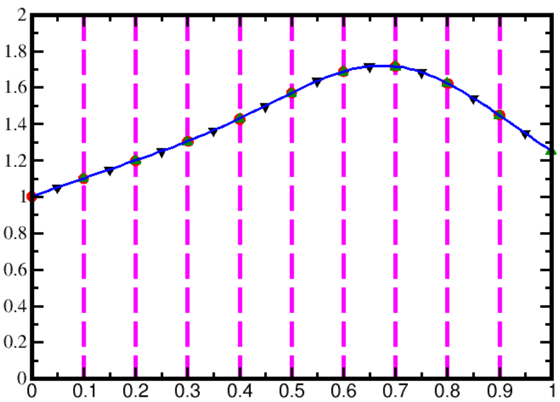

Figure 3.2: Different rectangular integration rules. In this example, we have ten rectangles whose area we sum to approximate the integral $\int_0^1 f(x)\,dx$ ($f(x)$ in blue). The left-point rule, takes the values of the functions at the red circles for each rectangle. The right point rule takes the values with the green triangles, while the midpoint rule takes the black triangular values. In the limit as the step size goes to zero, all rules will give the same answer, but their results differ for $\Delta x \neq 0$.

$x_i^{\text{right}} = i\Delta x$. The midpoint rule, averages the two and is $x_i^{\text{mid}} = \left(i - \frac{1}{2}\right)\Delta x$. In all cases $1 \leq i \leq n$ ($n = 10$ in the figure). These first rules are rectangular integration rules. Images most effectively illustrate the different methods, as can be seen in the corresponding Figs. 3.3-3.5.

The trapezoidal rule uses trapezoids to fit the curve (red trapezoids). This result is exactly equivalent to a different set of rectangles centered at the gridpoints; in this case, for the first and last points, only one-half of the corresponding rectangle contributes.

The next to consider is the so-called Simpson's rule, which approximates the integral via summing with weights that exactly integrate constant, linear, and quadratic functions. It can also be thought of as approximating the function with a quadratic for every sequence of three adjacent points on the grid. We will not draw a figure for this, but you can certainly imagine what it looks like. As with the trapezoidal rule, the construction simplifies, and can be thought of as integration over rectangles with the weights alternating

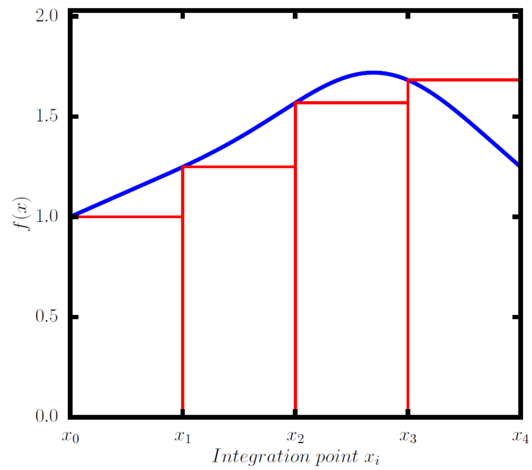

Figure 3.3: Left-hand integration rule with four points, given by $\int_{x_0}^{x_4} f(x)dx \approx \Delta x \left[f(x_0) + f(x_1) + f(x_2) + f(x_3)\right]$.

from 4/3 to 2/3 with the endpoints given by 1/3 again:

$$\int_{x_0}^{x_5} f(x)dx \approx \Delta x \left[\frac{1}{3}f(x_0) + \frac{4}{3}f(x_1) + \frac{2}{3}f(x_2) + \frac{4}{3}f(x_3) + \frac{1}{3}f(x_4)\right] \quad (3.29)$$

The sum alternates $\frac{4}{3}$ weight and $\frac{2}{3}$ weight, with $\frac{1}{3}$ weight on the endpoints. The generalization of Simpson's rule to higher polynomials is called Romberg integration. Many prefer this type of extrapolation technique to other methods. One can think of it as a technique that tries to extrapolate all the way to $\Delta x \to 0$.

There is one other technique for integration called Gaussian integration where the abscissae and weights are determined from a prescribed formula that exactly integrates a weight function times a polynomial of some degree. In this case, the spacing of the grid points is not uniform and it changes for every point as the number of points in the sum changes. This can make it inconvenient for computation and determining accuracy when one computes for different numbers of grid points. The reason why, is for grids that are evenly spaced, we simply double the number of points. Then half of the old grid points are on the new grid and we do not need to recalculate the function at those points. This never holds with Gaussian integration techniques. They are used, however, because if you have an integral of the form of a Gaussian

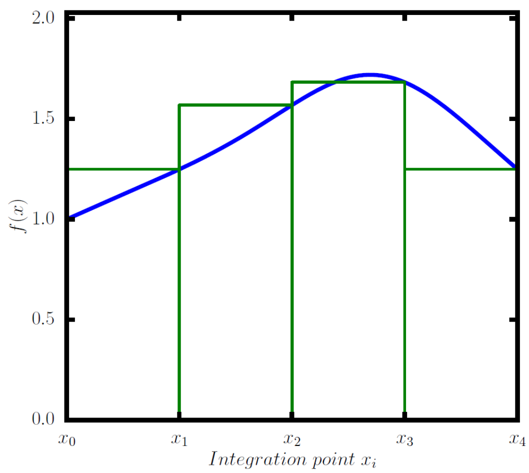

Figure 3.4: Right-hand integration rule with four points, given by $\int_{x_0}^{x_4} f(x)dx \approx \Delta x\,[f(x_1) + f(x_2) + f(x_3) + f(x_4)]$.

integration weight function, this tailor-made approach is likely to be superior. Calculating the weights and the gridpoints, however, is complicated.

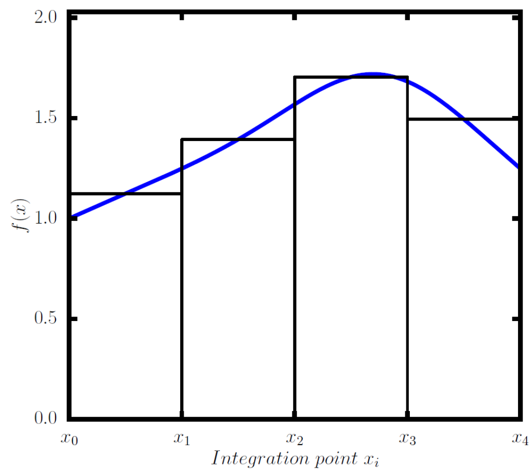

Figure 3.5: Midpoint integration rule with four points, given by $\int_{x_0}^{x_4} f(x)dx \approx \Delta x \left[f\left(\frac{x_0+x_1}{2}\right) + f\left(\frac{x_1+x_2}{2}\right) + f\left(\frac{x_2+x_3}{2}\right) + f\left(\frac{x_3+x_4}{2}\right)\right]$.

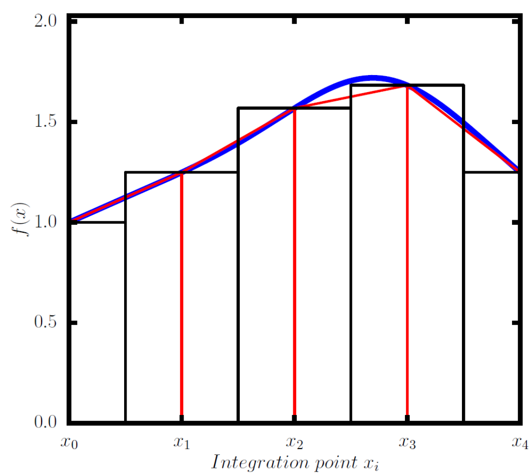

Figure 3.6: Trapezoidal integration rule with four points. The red trapezoids show the integration following the direct rule. It is equivalent to the black rectangles with the first and last counted half. The rule is given by $\int_{x_0}^{x_4} f(x)dx \approx \Delta x \left[\frac{1}{2}f(x_0) + f(x_1) + f(x_2) + f(x_3) + \frac{1}{2}f(x_4)\right]$.