8 Lecture #6: Wednesday, March 4th, 2026

8.1 Numerical derivation

Let us develop our first genuine numerical method. Consider the following problem: given a function f and a point a, we would like to compute $f'(a)$. A standard Calculus course cannot fully help us here because the function f does not necessarily come with an explicit formula. Let us consider a situation where this happens. Suppose that $f(t)$ describes the temperature in a room as we move through it, so that the temperature changes with t. We would like to determine $f'(a)$ at the point $t = a$. Since the system is too complex and involves many variables, there is no practical way to obtain an explicit formula for f. Nevertheless, it is still useful to estimate how the temperature changes in the room, which naturally leads us to a numerical approach.

Let us consider the definition of derivative. We know that

$$f'(a) = \lim_{h \to 0} \left(\frac{f(a+h) - f(a)}{h} \right).$$

Then, for a very small $h > 0$[¶], we can write $f'(a) \approx \frac{f(a+h)-f(a)}{h}$, which is called the **forward difference** approximation (see Figure 31).

Example 8.1. Let us look at $[e^x]'(0)$. Of course, we already know its exact value, but let us use the previous ideas to approximate it (see Figure 27). Notice that as h becomes smaller, the ratio $\frac{f(a+h)-f(a)}{h}$ gets closer to 1, which is the value of the derivative of the exponential function at 0.
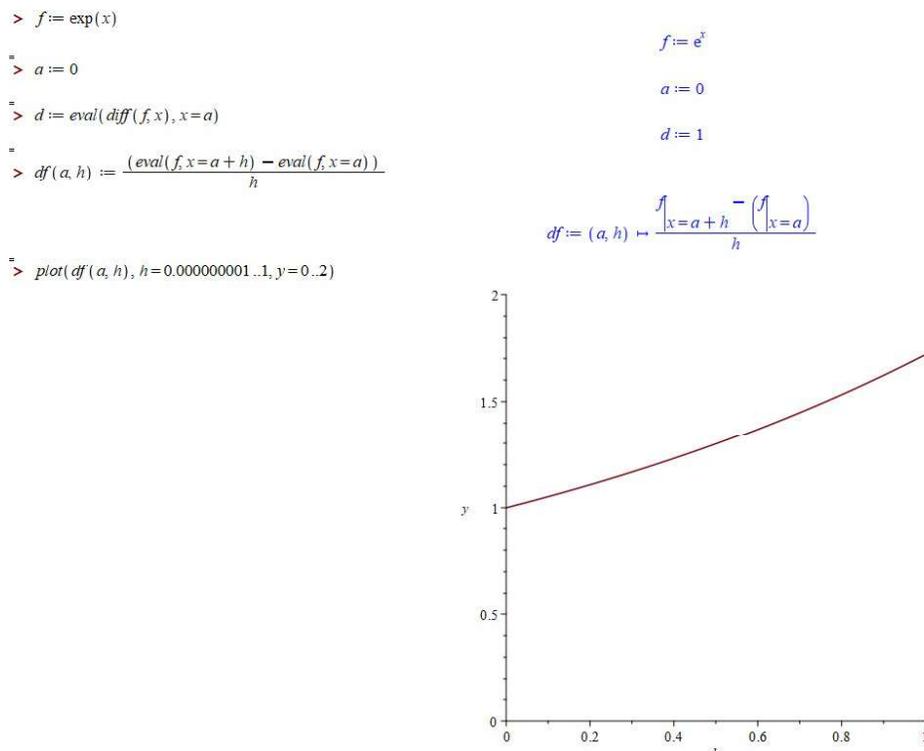

Figure 27: Graph of the difference $\frac{f(a+h)-f(a)}{h}$ where $f(x) = e^x$ and $a = 0$.

[¶]As an indicator of quality, h is always taken as a positive number in Numerical Analysis.

How much can we trust this procedure? In other words, what is the error of this method? Answering this question is our first important step. The plot of the error is shown in Figure 28.

> plot(d − df(a, h), h = 0.000000001 ..1)

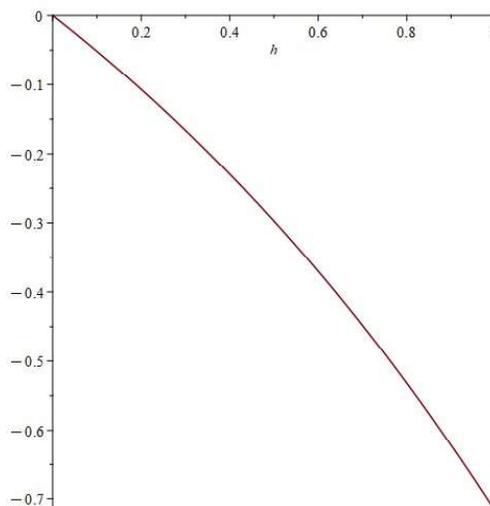
Figure 28: The graph represents the error of the method. Here $d = 1$ and $d(f, a) = \frac{f(a+h)-f(a)}{h}$.

Notice that, in this case, the error is negative. Since the error refers to the derivative, we have, by using the definition of error, that

$$E_{f'(a)}(h) =: E_h = x - \hat{x} = f'(a) - \frac{f(a + h) - f(a)}{h}.$$

As shown in Figure 27, all the approximations are greater than 1, which explains the negative values observed in the error curve in Figure 28. Notice now that if we zoom in and take values of h between 0.000000001 and 0.1, the curve appears almost flat, as shown in Figure 29. This shows that the error behaves as a straight life for small values of h.

> plot(d − df(a, h), h = 0.000000001 ..0.1)

>
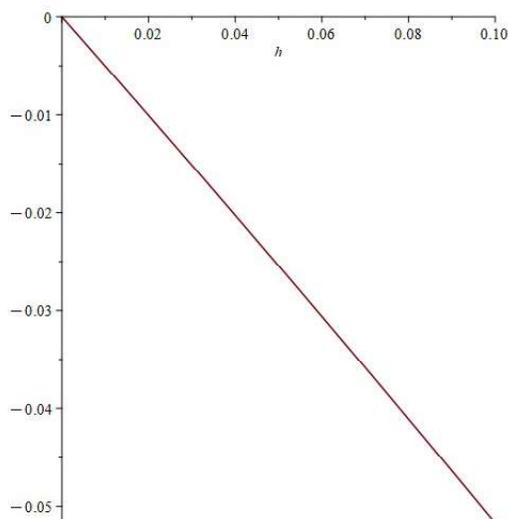
Figure 29: Now the graph has a smaller range on h.

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Let us see mathematically that the error indeed behaves like Example 8.1. Let us consider the Taylor expansion of f at a. Let us use the O-notation to write

$$f(a+h) = f(a) + f'(a)h + \frac{1}{2}f''(a)h^2 + O(h^3).$$

This means that

$$\frac{f(a+h) - f(a)}{h} = f'(a) + \frac{1}{2}f''(a)h + O(h^2).$$

Therefore, the formula of the error is given by

$$E_h = f'(a) - \frac{f(a+h) - f(a)}{h} = -\frac{1}{2}f''(a)h + O(h^2)$$

(notice that $-O(h^2) = O(h^2)$). We can conclude that $E_h = O(h)$, which agrees with our example, since the approximation is linear in h. This means that there exists a constant $C > 0$ such that $|E_h| \leqslant C \cdot h$ for sufficiently small values of h. Using a more precise notation, we can write $E_h \sim -\frac{1}{2}f''(a)h$. In particular, in Example 8.1, we have $f''(x) = e^x$, and therefore $f''(0) = 1$, which gives $E_h \sim -\frac{1}{2}h$. This behavior is illustrated in Figure 30; as we approach zero, the two curves become nearly indistinguishable.
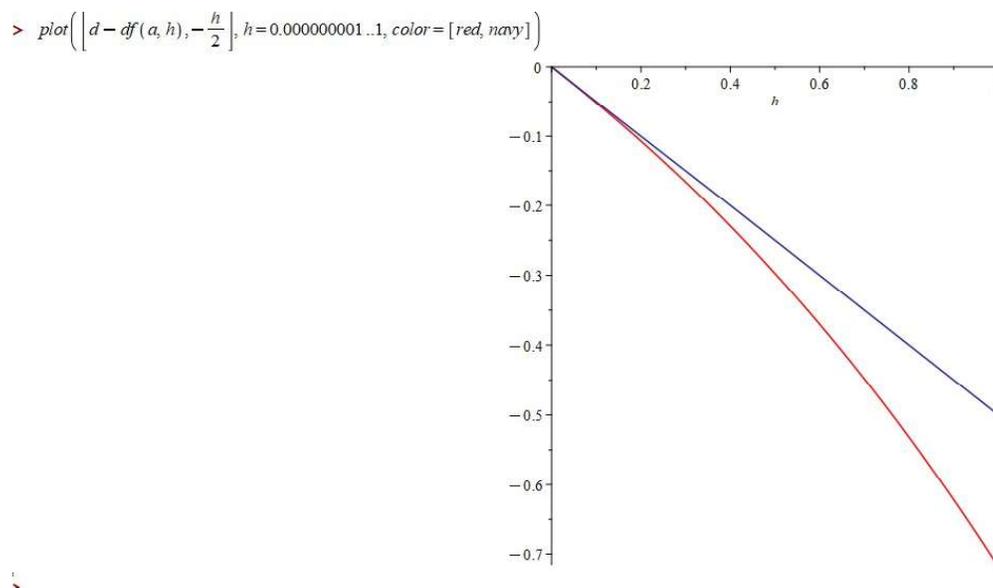

Figure 30: Comparison between the error E_h and $-\frac{h}{2}$.

An important issue about the forward difference is that it is biased[||]. Notice that in the Figure 27 it always overshoots the correct answer. The forward difference approximation can overshoot the true derivative because it replaces the tangent slope at a with the slope of a secant line joining the points $(a, f(a))$ and $(a+h, f(a+h))$. When the function is convex near a (that is, $f''(a) > 0$), the graph bends upward, so the slope of the function increases as we move to the right. Since the secant line uses the value at the future point $a+h$, where the function is already steeper, its slope becomes larger than the instantaneous slope at a. As a result, the forward difference produces a systematic overestimate (overshoot) of the derivative (see Figure 31).

[||] A biased method (or biased numerical method) is a method whose approximation has a systematic error in one direction; that is, it tends to consistently overestimate or underestimate the exact value.
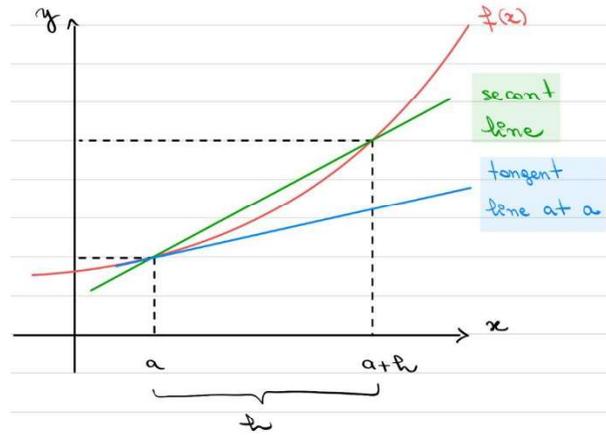
Figure 31: Forward difference method.

The **backward difference** approximation estimates, on the other hand, the derivative at a point a by using information from a previous point, replacing the tangent slope with the slope of the secant line joining $(a - h, f(a - h))$ and $(a, f(a))$, giving the formula $\frac{f(a)-f(a-h)}{h}$. Geometrically, it measures how the function has changed when moving toward a from the left, so it uses only past data (see Figure 32).
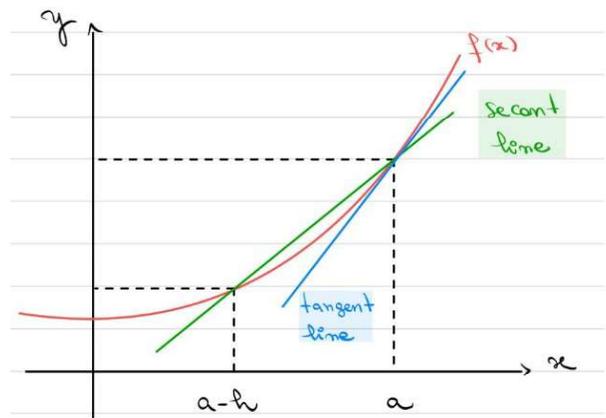

Figure 32: Backward difference method.

In this case, the backward difference gives the following approximation:
$$f'(a) \approx \frac{f(a) - f(a - h)}{h}.$$

When we analyze the quality of this approximation, we find that it has essentially the same order of error as the forward difference method, but now the approximation typically undershoots the true value. This means that the reliability of both methods are basically the same.

What if we take the average** of the forward and backward approximations? In that case, we obtain
$$f'(a) \approx \frac{f(a + h) - f(a - h)}{2h}.$$

The **average (also called the **arithmetic mean**) of two numbers is the value exactly halfway between them, that is, the average between x and y is given by $\frac{x+y}{2}$.

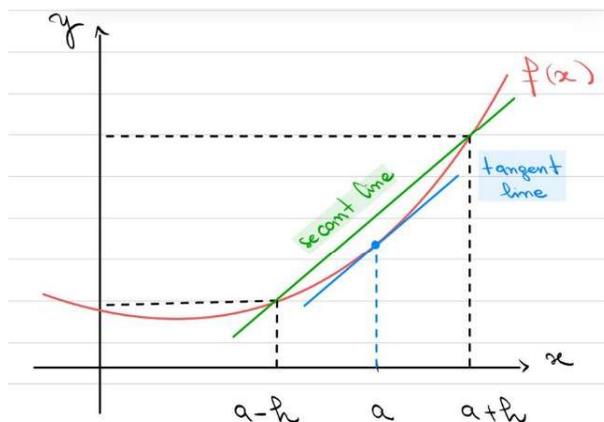This is called the **central difference** approximation (see Figure 33).

Figure 33: Central difference method.

How can we calculate the error of this approximation? In this case, we have that

$$f(a + h) = f(a) + f'(a)h + \frac{1}{2}f''(a)h^2 + \frac{1}{3!}f'''(a)h^3 + O(h^4)$$

and

$$f(a - h) = f(a) - f'(a)h + \frac{1}{2}f''(a)h^2 - \frac{1}{3!}f'''(a)h^3 + O(h^4).$$

We would like to combine the values $f(a)$, $f(a+h)$, and $f(a-h)$ to obtain the best possible approximation for $f'(a)$. To do this, we look for constants A, B, and C such that, using the Taylor expansions of $f(a+h)$ and $f(a-h)$, we have

$$Af(a) + Bf(a + h) + Cf(a - h) = (A + B + C)f(a) + (B - C)f'(a)h + \frac{1}{2}(B + C)f''(a)h^2$$

$$+ \frac{1}{3!}(B - C)f'''(a)h^3 + O(h^4).$$

Dividing by h gives

$$\frac{Af(a) + Bf(a + h) + Cf(a - h)}{h} = \frac{1}{h}(A + B + C)f(a) + (B - C)f'(a) + \frac{1}{2}(B + C)f''(a)h$$

$$+ \frac{1}{3!}(B - C)f'''(a)h^2 + O(h^3).$$

Since $1/h$ becomes unbounded as h gets small, we first require $A+B+C = 0$ to eliminate that term. Next, because we want an approximation of $f'(a)$, we impose $B - C = 1$. Finally, to obtain the most accurate approximation possible using three constants, we also require $B + C = 0$, which cancels the $f''(a)h$ term and therefore reduces the leading error. So, we need to solve

$$\begin{cases} A + B + C = 0, \\ B - C = 1, \\ B + C = 0. \end{cases}$$

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This gives $A = 0$, $B = \frac{1}{2}$, and $C = -\frac{1}{2}$. Therefore,

$$\frac{\frac{1}{2}f(a+h) - \frac{1}{2}f(a-h)}{h} = f'(a) + \frac{1}{3!}f'''(a)h^2 + O(h^3).$$

Equivalently,

$$\frac{f(a+h) - f(a-h)}{2h} = f'(a) + \frac{1}{3!}f'''(a)h^2 + O(h^3).$$

This shows that, if we use the three data values $f(a)$, $f(a+h)$, and $f(a-h)$, the best approximation for the derivative $f'(a)$ is given by the central difference formula. Moreover, we have obtained the error of this method, which is given by

$$E_h \sim -\frac{1}{6}f'''(a)h^2 + O(h^3) = O(h^2).$$

Hence, the central difference method has a significantly smaller error than both the forward and backward difference approximations. In Figure 34 we see the comparison between these three approximations. Notice also that the blue curve, which represents the central difference error, stays much closer to zero than the other two curves.
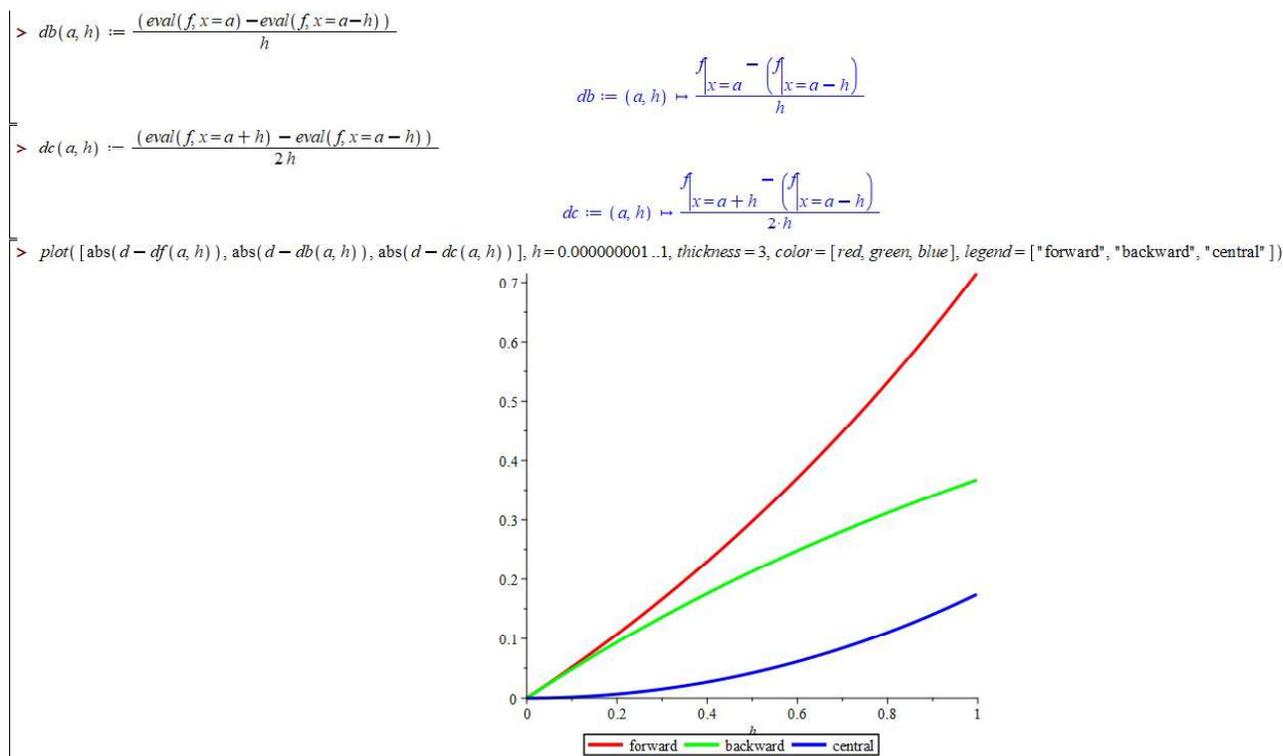

Figure 34: Comparison of the errors yield by the forward, backward and central differences.

In Figure 35, we reduce the range and can see more explicitly how much better the central difference method behaves.
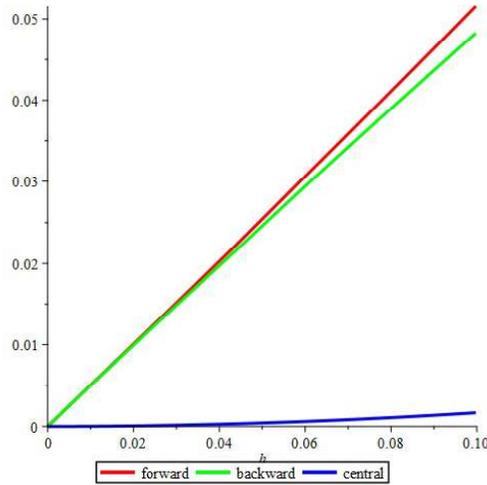
Figure 35: Comparison between the forward, backward and central differences.

To sum up, we have the following result. Let us notice that the approximation for $f''(a)$ below can be obtained in a similar way to what we have done for $f'(a)$.

Fact 8.2. Consider a function f that is three times continuously differentiable on some neighborhood of a point a. Then the following approximation formulas are true as $h \to 0$.

★ (forward difference) $f'(a) = \dfrac{f(a + h) - f(a)}{h} + O(h)$.

★ (backward difference) $f'(a) = \dfrac{f(a) - f(a - h)}{h} + O(h)$.

★ (central difference) $f'(a) = \dfrac{f(a + h) - f(a - h)}{2h} + O(h^2)$.

★ $f''(a) = \dfrac{f(a + h) + f(a - h) - 2f(a)}{h^2} + O(h^2)$.

For the last expression, we need to assume that f is four times continuously differentiable on some neighborhood of a.

8.2   Numerical integration

In the same spirit as the previous section, we now seek an approximation for the quantity

$$I = \int_a^b f(x)dx \tag{15}$$

when the function f is not necessarily given by an explicit formula. Moreover, there are integrals such as

$$\int_a^b e^{-x^2}dx$$

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that cannot be computed in closed form. To address these situations, we will introduce numerical methods known as **quadrature methods**. To do this, the first step is to divide the interval $[a, b]$ into $n \in \mathbb{N}$ equal subintervals (that is, a partition), each of length

$$h = \frac{b-a}{n}.$$

This quantity h is called the **step size**. Let us write this partition as $\{a = x_0 < x_1 < x_2 < \ldots < x_n = b\}$. Of course, once the partition is fixed, we can consider the values $f(x_0), f(x_1), f(x_2), \ldots, f(x_n)$. We will use these values to construct an approximation of the integral (15). For instance, we may consider the rectangles determined by the left endpoints and use them to approximate the integral, as illustrated in Figure 36 and the formula would go as

$$I \approx hf(x_0) + hf(x_1) + \ldots + hf(x_{n-1}).$$

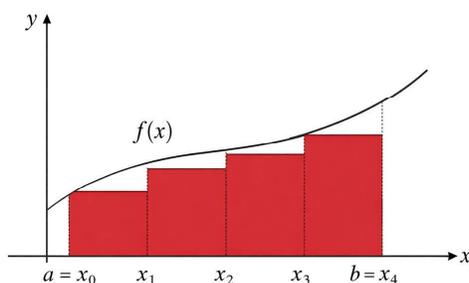This approximation is called the **left rectangle method**.

Figure 36: Approximation of the integral using the left-side rectangles.

Example 8.3. Let us calculate $I = \int_1^9 \ln(x)dx$. Notice that this integral can be determined by parts. However, let us use the left rectangle method. Take $n = 4$. Then, the step-size is given by

$$h = \frac{9-1}{4} = 2$$

as in the Figure 37.

Figure 37: Interval $[1, 9]$ and step-size $h = 2$.
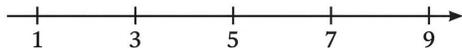
Then, we can factor out 2 in the formula and obtain

$$I \approx 2 \cdot \left[\ln(1) + \ln(3) + \ln(5) + \ln(7)\right].$$

Why not trying the right-side rectangles? In this case, the formula would be

$$I \approx hf(x_1) + hf(x_2) + \ldots hf(x_n) = h(f(x_1) + f(x_2) + \ldots + f(x_n)).$$

This is the **right-rectangles method**. We have the following definition.

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Definition 8.4. Let f be an integrable function on an interval $[a, b]$. For $n \in \mathbb{N}$, denote

$$h = \frac{b-a}{n}$$

and consider the points $x_i = a + ih$. By the **method of left rectangles** of **rectangle rule** with left endpoints for estimating the integral $\int_a^b f(x)dx$ we mean the formula

$$R_l(n) = h \sum_{i=0}^{n-1} f(x_i) = h[f(x_0) + \ldots + f(x_{n-1})],$$

By the **method of right rectangles** or **rectangle rule** with right endpoints for estimating the integral $\int_a^b f(x)dx$ we mean the formula

$$R_r(n) = h \sum_{i=1}^{n} f(x_i) = h[f(x_1) + \ldots + f(x_n)].$$

Example 8.5. For the same integral as in Example 8.3, we also can use the right rectangles to get the following approximation

$$\int_1^9 \ln(x)dx \approx 2[\ln(3) + \ln(5) + \ln(7) + \ln(9)].$$

Example 8.6. Let us see what happens when we apply these two methods using Maple to approximate

$$\int_0^{\frac{\pi}{2}} \sin(x)dx = 1.$$

The right-endpoint rectangles are shown on the right in Figure 38. Notice that this approximation over-shoots the true value while the left rectangles undershoots the real value as we can see on the left in the same picture.
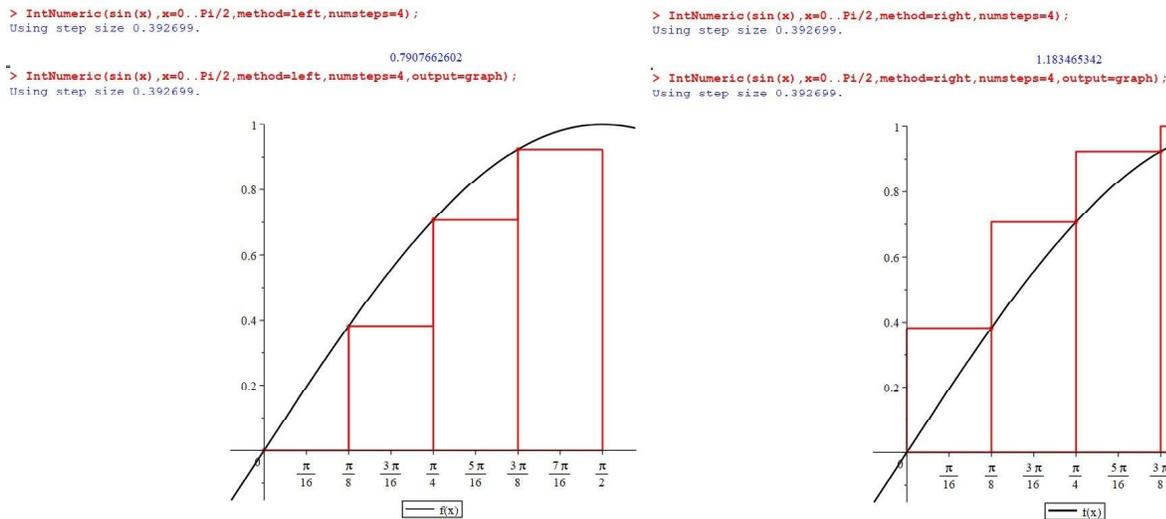

Figure 38: The left and right rectangles method, respectively.

These error estimates show that both the left- and right-rectangle rules have essentially the same accuracy: the error is proportional to the step size h (or equivalently to $1/n$). In particular, the error is bounded by a constant depending on the interval length $(b - a)$ and on $M_1 = \max_{x \in [a,b]} |f'(x)|$, which measures how rapidly the function changes. Geometrically, this means that the more the function varies (the larger its slope), the less accurate the rectangular approximation becomes. The bound also shows that refining the partition improves the approximation linearly: if we halve h, the error is approximately halved. Hence, both rectangle methods are **first-order** (see Definition 8.8 below) numerical schemes with comparable error behavior, differing mainly in whether they tend to overestimate or underestimate the true integral. We sum up these ideas in the following theorem.

Theorem 8.7. Consider a function f on an interval $[a, b]$. Denote by $M_1 = \max_{x \in [a,b]} |f'(x)|$. If we approximate the integral $I = \int_a^b f(x)dx$ using a rectangle rule, then we have the following error estimates:

$\star$ $|I - R_l(n)| \leqslant \dfrac{1}{2}(b - a)^2 M_1 \dfrac{1}{n} = \dfrac{1}{2}(b - a)M_1 h.$

$\star$ $|I - R_r(n)| \leqslant \dfrac{1}{2}(b - a)^2 M_1 \dfrac{1}{n} = \dfrac{1}{2}(b - a)M_1 h.$

Notice then that the rectangle rules produces errors $E_h = O(h)$. This means that its order is 1 as we can see in the next definition. In a different notation, we can write it as $E_h \sim ch$ for some constant $c > 0$.

Definition 8.8. We say that a method I_n for approximating an integral is of **order** p for $p \in \mathbb{N}$, provided that for every function f on an interval $[a, b]$ there is $C > 0$ such that

$$\left| \int_a^b f(x)dx - I_n \right| \leqslant C\frac{1}{n^p}.$$

That is, $|I - I_n|$ is $O(h^p)$ as $h \to 0^+$.

8.3 The trapezoid method

So far we have introduced two methods for approximating an integral, and we have seen that both are first-order methods (see Theorem 8.7). It is now natural to look for a better approximation. As mentioned earlier, the left rectangle method typically undershoots the true value of the integral, while the right rectangle method overshoots it. A natural idea is therefore to take the average of the two methods. Doing so leads to the approximation

$$I \approx \frac{1}{2}h\left[f(x_0) + 2f(x_1) + 2f(x_2) + \ldots + 2f(x_{n-1}) + f(x_n)\right].$$

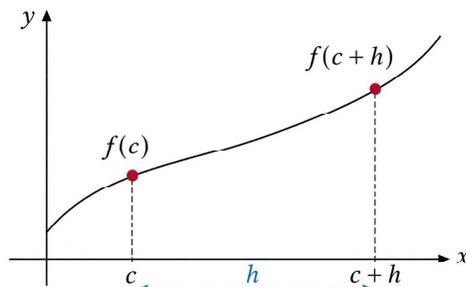Let us consider just one panel in our partition as in Figure 39.

Figure 39: Only one panel.

In this case, the average of the left and right rectangle methods is

$$\frac{1}{2}h \cdot [f(c) + f(c+h)] = h \cdot \frac{f(c) + f(c+h)}{2}.$$

In other words, this expression can be interpreted as the area of a rectangle with base h and height equal to the average value $\frac{f(c)+f(c+h)}{2}$. Geometrically, this is equivalent to the area of a trapezoid with height h and parallel sides of lengths $f(c)$ and $f(c+h)$. At first glance, this provides a much better approximation and suggests that the method may have a higher order of accuracy. Notice, therefore, that

$$I \approx h \cdot \frac{f(x_0) + f(x_1)}{2} + h \cdot \frac{f(x_1) + f(x_2)}{2} + \ldots + h \cdot \frac{f(x_{n-1}) + f(x_n)}{2}$$

which is called the **trapezoid method** (see Figure 40).

Definition 8.9. Let f be an integrable function on an interval $[a, b]$. For $n \in \mathbb{N}$, denote $h = \frac{b-a}{n}$ and consider the points $x_i = a + ih$. By the **trapezoid rule** for estimating the integral $\int_a^b f(x)dx$ we mean the formula

$$T(n) = \frac{1}{2} \cdot h \cdot \left[\sum_{i=0}^{n-1} f(x_i) + \sum_{i=1}^{n} f(x_i) \right] = \frac{1}{2} \cdot h \cdot \left[f(x_0) + \sum_{i=1}^{n-1} 2f(x_i) + f(x_n) \right].$$

Example 8.10. Let use the trapezoid method to get an approximation for

$$I = \int_1^9 \ln(x)dx.$$

Let us consider $n = 4$ and then $h = \frac{9-1}{4} = 2$. Then,

$$I \approx \frac{1}{2} \cdot 2 \cdot [\ln(1) + 2\ln(3) + 2\ln(5) + \ln(9)].$$

In the example for Figure 40, if one uses the code

IntNumeric(sin(x),x=0..Pi/2,method=trapezoid,numsteps=4,output=totalerror);

one will realize that the error is 0.0128841989, which is much smaller than both right and left rectangle methods. In fact, we have the following result.

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Theorem 8.11. Consider a function f on an interval $[a, b]$. Denote $M_2 = \max_{x \in [a,b]} |f''(x)|$. If we approximate the integral $I = \int_a^b f(x)dx$ using the trapezoid rule, then we have the following error estimate:

$$|I - T(n)| \leqslant \frac{1}{12}(b-a)^3 M_2 \frac{1}{n^2} = \frac{1}{12}(b-a)M_2 h^2$$

for $h = \frac{b-a}{n}$.

In particular, this means that $E_h = O(h^2)$, that is, $E_h \sim c \cdot h^2$ for some $c > 0$. In other words, the trapezoid method is of order 2.
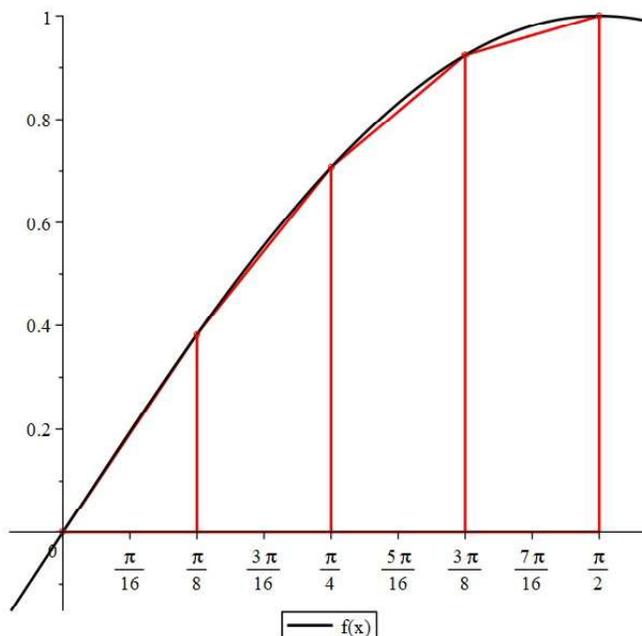

Figure 40: Once again the example with $f(x) = \sin(x)$ between 0 and $\frac{\pi}{2}$ using the trapezoid method.

8.4   The Simpson method

The Simpson method is a numerical technique used to approximate definite integrals by replacing the function on small subintervals with quadratic polynomials instead of straight lines. Unlike the rectangle or trapezoidal rules, which use constant or linear approximations, Simpson's method fits a parabola through nearby points of the graph, producing a much more accurate estimate of the area under the curve. As a result, it achieves a higher order of accuracy and is especially effective when the function is smooth.

However, after dividing the interval $[a, b]$ into subintervals of equal length, there are infinitely many polynomials that could pass through, for example, the points $(x_i, f(x_i))$ and $(x_{i+1}, f(x_{i+1}))$. To avoid this ambiguity, we assume that the number of subintervals n in the step size $h = \frac{b-a}{n}$ is even. We then consider three consecutive points, $(x_{i-1}, f(x_{i-1}))$, $(x_i, f(x_i))$, and $(x_{i+1}, f(x_{i+1}))$. Through these three points there exists a unique quadratic polynomial, that is, a parabola, which is used to approximate the function locally.

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Definition 8.12. Let f be an integrable function on an interval $[a, b]$. For $n \in \mathbb{N}$, n even, denote $h = \frac{b-a}{n}$ and consider points $x_i = a + ih$. By the **Simpson rule** for estimating the integral $\int_a^b f(x)dx$ we mean the formula

$$S(n) = \frac{1}{3}h\left[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \ldots + 4f(x_{n-1}) + f(x_n)\right].$$

Indeed, this is a better approximation compared to the others as we have the following result which tell us about the order of this method.

Theorem 8.13. Consider a function f on an interval $[a, b]$. Denote $M_4 = \max_{x \in [a,b]} |f''''(x)|$. If we approximate the integral $I = \int_a^b f(x)dx$ using the Simpson rule, then we have the following error estimate

$$|I - S(n)| \leqslant \frac{1}{180}(b-a)^5 M_4 \frac{1}{n^4} = \frac{1}{180}(b-a)M_4 h^4$$

for $h = \frac{b-a}{n}$.