

Numerical Methods

§10.1. Taylor Approximation

Suppose that f is a function defined in a neighborhood of a point c , and suppose that f has derivatives of all orders near c . In Chapter 9.5 we introduced the Taylor polynomials for f :

Definition 10.1 *The Taylor polynomial of degree n of f , centered at c is*

$$(10.1) \quad (T_c^{(n)} f)(x) = \sum_{k=0}^n \frac{f^{(k)}(c)}{k!} (x-c)^k.$$

We discovered these polynomials by looking for the best polynomial approximation to f .

Proposition 10.1 *The Taylor polynomial $T_c^{(n)} f$ is the polynomial of degree n or less which approximates f near c to n th order.*

In this section, we shall show how the Taylor polynomials effectively approximate the function f . Thus we need information on the error incurred by these approximations. This also was given in the previous section:

Proposition 10.2 *Suppose that f is differentiable to order $n+1$ in the interval $[c-a, c+a]$ centered at the point c . Then the error in approximating f in this interval by its Taylor polynomial of degree n , $T_c^{(n)} f$ is bounded by*

$$(10.2) \quad \frac{M_{n+1}}{(n+1)!} |x-c|^{n+1},$$

where M_{n+1} is a bound of the values of $f^{(n+1)}$ over the interval $[c-a, c+a]$. To be precise, we have the inequality

$$(10.3) \quad |f(x) - T_c^n f(x)| \leq \frac{M_{n+1}}{(n+1)!} |x-c|^{n+1} \quad \text{for all } x \text{ between } c-a \text{ and } c+a.$$

Before using this estimate, let us see how it comes about. To simplify the notation, we shall take c to be the origin.

First, a preliminary step:

Lemma. Suppose that $f(0) = 0, f'(0) = 0, \dots, f^{(n)}(0) = 0$. Then

$$(10.4) \quad |f(x)| \leq \frac{M_{n+1}}{(n+1)!} |x|^{n+1}.$$

Let's show the case $n = 1$. We have $|f''(s)| \leq M_2$ for all $s, 0 \leq s \leq x$. So, for any $t, 0 \leq t \leq x$, we have

$$(10.5) \quad |f'(t)| = \left| \int_0^t f''(s) ds \right| \leq \int_0^t |f''(s)| ds \leq M_2 \int_0^t ds \leq M_2 t.$$

But now,

$$(10.6) \quad |f(x)| = \left| \int_0^x f'(t) dt \right| \leq \int_0^x |f'(t)| dt \leq \int_0^x M_2 t dt \leq M_2 \frac{x^2}{2}.$$

Of course, the same argument works for x negative, we just have to be careful with the signs.

The argument for any n just bootstraps from this, proceeding from the estimate for $n - 1$ to the estimate for n (this is called a *proof by induction*). Suppose we have gotten to the $(n - 1)$ th case. Then the lemma applies (at $n - 1$) to the derivative f' ; so we know that

$$(10.7) \quad |f'(t)| \leq \frac{M_{n+1}}{n!} |t|^n \quad \text{for all } t \text{ in the interval } [-a, a].$$

(We have M_{n+1} because the n th derivative of f' is the $(n + 1)$ th derivative of f). Now we argue independently on each side of 0: for $x > 0$:

$$(10.8) \quad \begin{aligned} |f(x)| &= \left| \int_0^x f'(t) dt \right| \leq \int_0^x |f'(t)| dt \leq \int_0^x \frac{M_{n+1}}{n!} t^n dt \\ &\leq \frac{M_{n+1}}{n!} \frac{t^{n+1}}{n+1} \Big|_0^x = \frac{M_{n+1}}{(n+1)!} |x|^{n+1}. \end{aligned}$$

The argument for $x < 0$ is the same; just be careful with signs. Now that the lemma is verified, we go to the proposition itself. Let $g = f - T_c^{(n)} f$. Then g satisfies the hypotheses of the lemma. Furthermore, since $T_c^{(n)} f$ is a polynomial of degree n , its $(n + 1)$ th derivative is identically zero. Thus $g^{(n+1)}$ has the same bound, M_{n+1} . Applying the lemma to g , we have the desired result:

$$(10.9) \quad |f(x) - T_c^{(n)} f| \leq \frac{M_{n+1}}{(n+1)!} |x|^{n+1}.$$

If this error estimate converges to 0 as $n \rightarrow \infty$, then we saw that f is be represented by its *Taylor series*:

$$(10.10) \quad f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(c)}{n!} (x - c)^n$$

in the interval $[c - a, c + a]$.

Before doing some examples, let's review what has to be done. To use the Taylor polynomials to find approximate values to a function, we first have to find bounds M_n for the successive derivatives of the function. Then we have to calculate the values of

$$(10.11) \quad \frac{M_n}{n!} |x - c|^n$$

for successive values of n until we have found one which is within the desired error. Then we calculate using the Taylor polynomial of degree $n - 1$.

Example 10.1 Find \sqrt{e} to within an error of 10^{-4} . This is $e^{1/2}$, so we look at the function $f(x) = e^x$. Since $f^{(n)}(x) = e^x$ for all n , and the value $x = 1/2$ is within 1 of 0, we can use the Maclaurin series for e^x and the bounds $M_n = e^1$. Since 3 is more manageable than e , we take $M_n = 3$. Now we estimate the error at stage n which we'll call $E(n)$. We have, in this example

$$(10.12) \quad E(n) = \frac{3}{n!} \left(\frac{1}{2}\right)^n.$$

$$(10.13) \quad n = 1: \quad E(1) = \frac{3}{2}$$

$$(10.14) \quad n = 2: \quad E(2) = \frac{3}{2} \frac{1}{4}$$

$$(10.15) \quad n = 3: \quad E(3) = \frac{3}{6} \frac{1}{8} = \frac{3}{48}$$

$$(10.16) \quad n = 4: \quad E(4) = \frac{3}{24} \frac{1}{16} = \frac{3}{384}$$

$$(10.17) \quad n = 5: \quad E(5) = \frac{3}{120} \frac{1}{32} = 7.8 \times 10^{-4}$$

$$(10.18) \quad n = 6: \quad E(6) = \frac{3}{720} \frac{1}{64} < 10^{-4}$$

Thus, we have our estimate to within 10^{-4} by taking the fifth Taylor polynomial:

$$(10.19) \quad T_0^5(e^x)(1/2) = 1 + \frac{1}{2} + \frac{1}{2} \frac{1}{4} + \frac{1}{6} \frac{1}{8} + \frac{1}{24} \frac{1}{16} + \frac{1}{120} \frac{1}{32} = 1.6487$$

Example 10.2 Find $\sin \pi/8$ to within an error of 10^{-3} .

Here we start with the Maclaurin series for $\sin x$:

$$(10.20) \quad \sin x = x - \frac{x^3}{6} + \frac{x^5}{120} + \dots$$

Since the derivatives of $\sin x$ alternate between $\pm \sin x$ and $\pm \cos x$, we may take $M_n = 1$ for all n . We need to choose n large enough that the Taylor error estimate $E(n)$ satisfies

$$(10.21) \quad E(n) = \frac{1}{n!} \left(\frac{\pi}{8}\right)^n < \frac{1}{2} 10^{-3}.$$

$$(10.22) \quad n = 1: \quad E(1) = \frac{\pi}{8} = .3927$$

$$(10.23) \quad n = 2: \quad E(2) = \frac{1}{2} \left(\frac{\pi}{8}\right)^2 = .077$$

$$(10.24) \quad n = 3: \quad E(3) = \frac{1}{6} \left(\frac{\pi}{8}\right)^3 = .010$$

$$(10.25) \quad n = 4: \quad E(4) = \frac{1}{24} \left(\frac{\pi}{8}\right)^4 = .0009$$

so we need only go to $n = 3$. The estimate is

$$(10.26) \quad T_0^3(\sin x)(\pi/8) = \frac{\pi}{8} - \frac{1}{6} \left(\frac{\pi}{8}\right)^2 = .3826$$

or $\sin(\pi/8) = .383$, correct to three decimal places.

Some Taylor series converge too slowly to get a reasonable approximation by just a few terms of the series. As a rule, if the series has a factorial in the denominator, this technique will work efficiently, otherwise, it will not.

Example 10.3 Use the Maclaurin series

$$(10.27) \quad \ln(1+x) = \sum_{n=1}^{\infty} (-1)^{n+1} \frac{x^n}{n}$$

to estimate $\ln(1+a)$ for $a > 0$ to within 4 decimal places.

First we calculate the successive derivatives of $f(x) = \ln(1+x)$ to obtain the bounds M_n . We have

$$(10.28) \quad f^{(n)}(x) = (-1)^{n-1} (n-1)! (1+x)^{-n}$$

so we can take $M_n = (n-1)!$. Thus we need, for $x = a$:

$$(10.29) \quad E(n) = \frac{(n-1)!}{n!} a^n = \frac{a^n}{n} < 10^{-4}.$$

If $a = 1/10$, then the estimate occurs at $n = 4$, so the first three terms will do. But if $a = 1/2$, we don't get this inequality until $n = 12$, so we'll need 11 terms of the series.

Figure 10.1

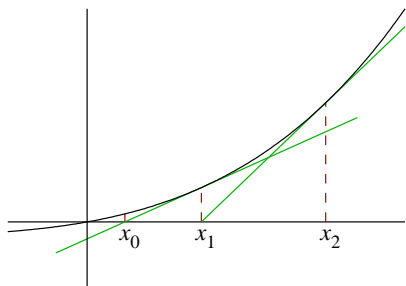
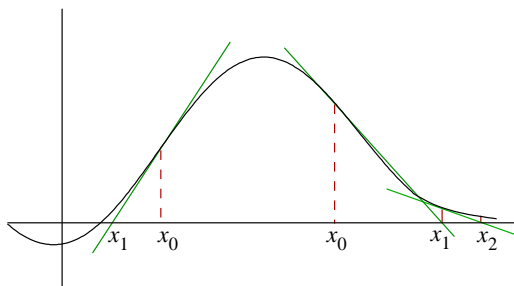


Figure 10.2



§10.2. Newton's method

Suppose that we want to estimate the solution of the equation $f(x) = 0$. If this is a linear equation, there is no problem: we just look for the point at which the line crosses the x -axis. Newton's idea is that, since the tangent line approximates the graph, why not take as the estimate the point at which the tangent line crosses the x -axis? Well, to make sense of this, let's start at some value x_0 and calculate $y_0 = f(x_0)$. If that is 0, then we're through. If not, let x_1 be the point at which the tangent line at (x_0, y_0) crosses the x -axis. That is our first approximation. If it is not good enough, replace x_0 with x_1 , and repeat the process, over and over again, until the result is good enough.

This process is illustrated in figure 10.1. However, it doesn't always work so well, as figure 10.2 shows. The important point is to start with a decent guess for x_0 , so that we start in a range of the function where the concavity of the curve forces convergence of these successive approximations.

Newton's method thus, is a technique for replacing an approximation by a better one. Suppose we start with the function $y = f(x)$, and have found an approximation $x = a$, with $f(a)$ (relatively) close to zero. The slope of the tangent line at $x = a$ is $f'(a)$, and the equation of the tangent line is $y - f(a) = f'(a)(x - a)$. This intersects the x -axis where $y = 0$, so we have

$$(10.30) \quad -f(a) = f'(a)(x - a) \quad \text{which has the solution} \quad x = a - \frac{f(a)}{f'(a)}$$

We now replace a by this value, and repeat the process. This is called a *recursion* given by the *recursion formula* (10.30). How do we know when we are within an error e of the solution? If the process is working, that is, if the successive approximations are getting closer and closer together, then we can stop as soon as they are within e of each other. If we have started with an estimate which is too far off, the process won't work at all, and we'll have to start with a better estimate.

Example 10.4 Find $\sqrt{8}$ correct to within 4 decimal places.

Here we want to find the root of the equation $f(x) = x^2 - 8 = 0$. Let's start with $x_0 = 3$. Since $f'(x) = 2x$, the next estimate is

$$(10.31) \quad x_1 = 3 - \frac{3^2 - 8}{2 \times 3} = 2.8333$$

We now use this in the recursion, and continue until we reach stability in the first 4 decimal places:

$$(10.32) \quad x_2 = 2.8333 - \frac{(2.8333)^2 - 8}{2 \cdot 2.8333} = 2.8284$$

$$(10.33) \quad x_3 = 2.8284 - \frac{(2.8284)^2 - 8}{2 \cdot 2.8284} = 2.8284,$$

which we conclude is the estimate accurate to 4 decimal places.

Before going on to other examples, we summarize the process: To solve $f(x) = 0$:

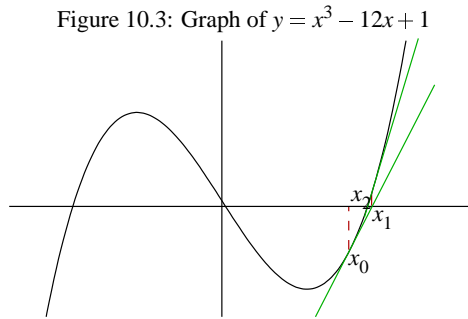
1. Calculate $f'(x)$.
2. Calculate the recursion relation

$$(10.34) \quad x' = x - \frac{f(x)}{f'(x)}.$$

3. Select a first estimate x_0 , so that $f(x_0)$ is small and $f'(x_0)$ is large.
4. Find x_1 from x_0 by taking $x = x_0$, $x' = x_1$ in the recursion relation.
5. Repeat step 4 until the successive estimates are no further from each other than the desired estimate.

Example 10.5 Find the solutions of $f(x) = x^3 - 12x + 1 = 0$ to three decimal places.

First we graph the function so as to make an intelligent first estimate. We have $f'(x) = 3x^2 - 12$, so the local maximum and minimum of $y = f(x)$ are at $(-2, 17)$, $(2, -15)$. At $x = 0$, $y = 1$, and the graph is as shown in figure 10.3. There are three solutions; one close to 0, another larger than 2, and a third less than -2.



First, find the solution near zero. We see from the graph that the derivative is well away from zero in a range including $x = 0$ and the solution, so we can take our first estimate to be $x_0 = 0$. Now we calculate successive estimates:

$$(10.35) \quad x_1 = 0 - \frac{1}{-12} = \frac{1}{12} = .08333$$

$$(10.36) \quad x_2 = .08333 - \frac{(.08333)^3 - 12(.08333) + 1}{3(.08333)^2 - 12} = .08338,$$

$$(10.37) \quad x_3 = .08338$$

so this solution is $x = .08338$ up to four decimal places. Now, to find the solution larger than 2, it will not do to take $x_0 = 2$, since the derivative is 0 there. But if we take $x_0 = 3$, we have $f'(3) = 15$, a nice large number, so the recursion should work. We find

$$(10.38) \quad x_1 = 3 - \frac{3^3 - 12(3) + 1}{3(3^2) - 12} = 3 - \frac{-8}{15} = 3.5333,$$

$$(10.39) \quad x_2 = 3.5333 - \frac{(3.5333)^3 - 12(3.5333) + 1}{3(3.5333)^2 - 12} = 3.4267$$

$$(10.40) \quad x_3 = 3.4215, \quad x_4 = 3.4215,$$

so this is the answer correct to four decimal places. In the same way, starting at $x_0 = -3$, we find the third solution.

Example 10.6 Solve $e^x = x + 2$ correct to three decimal places.

Here $f(x) = e^x - x - 2$, $f'(x) = e^x - 1$. Since the derivative is increasing, and greater than 1 at $x = 1$, and $f(1) < 0$, while $f(2) > 0$, a good first estimate will be any number between 1 and 2. So, take $x_0 = 1$. The recursion is

$$(10.41) \quad x' = x - \frac{e^x - x - 2}{e^x - 1} = \frac{e^x(x-1) + 2}{e^x - 1}.$$

We now calculate the successive estimates:

$$(10.42) \quad x_1 = 1.16395, \quad x_2 = 1.1464, \quad x_3 = 1.1462, \quad x_4 = 1.1462,$$

so this is the desired estimate. Notice that in this range, the derivative is not very large, so that the convergence is slower than in the preceding examples.

§10.3. Numerical Integration

We have learned techniques for calculating definite integrals which are based on finding antiderivatives of the function to be integrated. However, in many cases we cannot find an expression for the antiderivative, and these techniques will not lead to an answer. For example $f(x) = \sqrt{1+x^3}$. No formula for the integral exists in any integral tables. In such a case, we have to return to the definition of the integral, and approximate the definite integral by the approximating sums. To explain this, we first review the definition of the definite integral.

Definition 10.2 Let $y = f(x)$ be a function defined on the interval $[a, b]$. The definite integral is defined as follows. A partition of the interval is any increasing sequence

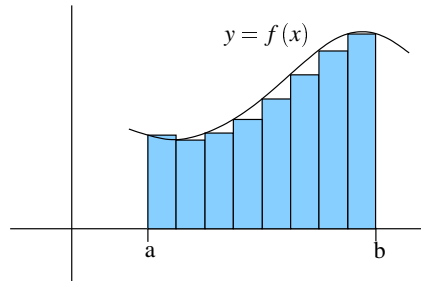
$$(10.43) \quad \{a = x_0 < x_1 < \cdots < x_{n-1} < x_n = b\}$$

of points in the interval. The corresponding approximating sum is

$$(10.44) \quad \sum_{i=1}^n f(x'_i) \Delta x_i$$

where Δx_i is the length $x_i - x_{i-1}$ of the i th interval, x'_i is any point on that interval, and Σ indicates that we add all these products together (see Figure 10.4).

Figure 10.4: Approximation to the area under a curve.



If these approximating sums approach a limit as the partition becomes increasingly fine (the lengths of the subdivisions go to zero), this limit is the *definite integral* of f over the interval $[a, b]$, denoted

$$(10.45) \quad \int_a^b f(x) dx .$$

Thus, we can approximate a definite integral by the sums (10.44). One way to accomplish this is the following. Pick an integer N , and divide the interval $[a, b]$ into N subintervals, all of size $(b - a)/N$. For each subinterval, evaluate the function at the right endpoint x_i , and form the sum

$$(10.46) \quad \sum_1^N f(x_i) \Delta x_i = \frac{(b-a)}{N} \sum_1^N f(x_i) \quad (\text{Approximating Rectangles})$$

Example 10.7 Let's find an approximate value for $\int_0^1 \sqrt{1+x^3} dx$ this way. Let's divide the interval into 10 subintervals. Then the sum (10.46) is

$$(10.47) \quad \begin{aligned} & \frac{1}{10} (\sqrt{1+(1/10)^3} + \sqrt{1+(2/10)^3} + \sqrt{1+(3/10)^3} + \cdots + \sqrt{1+(10/10)^3}) \\ &= \frac{1}{10} (1.0005 + 1.0040 + 1.0134 + 1.0315 + 1.0607 + 1.1027 + 1.1589 \\ &+ 1.2296 + 1.3149 + 1.4142) = 1.1330. \end{aligned}$$

Of course these calculations are tedious if done by hand, but, by computer - completely trivial. It is a good idea to try these using a spreadsheet, because there you get to follow the computation. If we take more subdivisions, we get a better approximation. For example, if we take $N = 100$ we get

$$(10.48) \quad \begin{aligned} & \frac{1}{100} (\sqrt{1+(1/100)^3} + \sqrt{1+(2/100)^3} + \sqrt{1+(3/100)^3} + \\ & \cdots + \sqrt{1+(100/100)^3}) = 1.113528, \end{aligned}$$

an apparently better approximation.

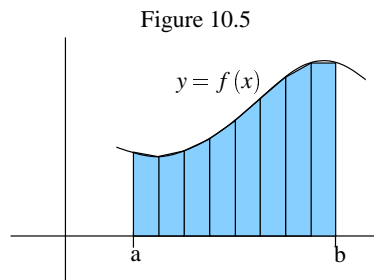
Example 10.8 Just to see how well this method is working, let us use it to approximate $\int_1^2 x^{1.4} dx$, which we know to be $(2^{2.4} - 1)/(2.4) = .1.782513 \dots$. Let's first take $N = 10$. The approximating sum is

$$(10.49) \quad \frac{1}{10} ((1.1)^{1.4} + (1.2)^{1.4} + (1.3)^{1.4} + \cdots + (2)^{1.4})$$

$$(10.50) \quad \frac{1}{10}(1.1427 + 1.2908 + 1.4438 + 1.6017 + 1.7641 + 1.9309 + 2.1020 + 2.2771 + 2.4562 + 2.6390) = 1.8648.$$

For $N = 100$ we obtain the estimate 1.790712, which is better, but not great.

We can improve this method by improving the estimate in each subinterval. First, note that we have estimated the integral in each subinterval by the area of the rectangle of height at the right endpoint. If instead we estimate this area using the trapezoid whose upper side is the line segment joining the two endpoints (see figure 10.5), it makes sense that this is a better estimate.



This comes down to

$$(10.51) \quad \frac{(b-a)}{2N}(f(a) + 2 \sum_1^{N-1} f(x_i) + f(b)) \quad (\text{Trapezoid Rule})$$

Going one step further, we might replace the upper curve by the best parabolic approximation. For N even, this leads to the rule

$$(10.52) \quad \frac{(b-a)}{3N}(f(a) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \cdots + 4f(x_{N-1}) + f(b)) \quad (\text{Simpson's Rule})$$

Let us now do the above examples using these two rules:

Example 10.9 The calculation of $\int_0^1 \sqrt{1+x^3} dx$ using the Trapezoidal rule and $N = 10$ gives us

$$(10.53) \quad \begin{aligned} & \frac{1}{20}(1 + 2(\sqrt{1+(1/10)^3} + \sqrt{1+(2/10)^3} + \sqrt{1+(3/10)^3} + \cdots \\ & \quad + \sqrt{1+(9/10)^3}) + \sqrt{2}) \\ & = \frac{1}{20}(1 + 2(1.0005 + 1.0040 + 1.0134 + \cdots + 1.2296 + 1.3149) \\ & \quad + 1.4142) = 1.0123. \end{aligned}$$

Example 10.10 Let's compare the estimates of $\int_0^1 x^{1.4} dx$ with these two new methods. First, with $N = 10$, and the trapezoid rule:

$$(10.54) \quad \frac{1}{20}(1 + 2((1.1)^{1.4} + (1.2)^{1.4} + (1.3)^{1.4} + \cdots + (1.9)^{1.4}) + 2^{1.4} =$$