Introduction

In this course we will be concerned with algorithms for performing three common Calculus tasks[1]:

1. Computation of integrals (quadrature).
2. Finding zeros of functions (root finding).
3. Solution of initial value problems.

However, Math 110 is not merely a course in computational methods—it is a course in Numerical Analysis! Therefore our main focus will be on the conceptual framework for numerical methods rather than the methods themselves.

By 'conceptual framework' I specifically mean *interpolation theory*. This, roughly speaking, is the theory about approximating complicated functions with simple functions. To see why interpolation is key to Numerical Analysis, consider the problem of one-dimensional quadrature: approximate $\int_a^b f(x)\,dx$. If we can approximate f with a polynomial p on $[a, b]$ then it is easy to approximate the integral of f, namely:

$$\int_a^b f(x)\,dx \approx \int_a^b p(x)\,dx.$$

The integral of a polynomial is, of course, trivial to compute. What is not trivial, however, is understanding how to properly derive the polynomial approximation *that ensures given accuracy*—that is what interpolation theory is largely about.

By the way, after three semesters of Calculus, the preceding paragraph should have rung some bells. Remember approximating functions of one variable with Taylor polynomials? In our new parlance, this was *Taylor interpolation*. If you happen to understand Taylor theory to the extent where you can derive the remainder of Taylor approximation, you may skip the following Calculus review. Otherwise, read on.

[1] If time allows, we will also talk about Numerical Linear Algebra. But no promises!

Rethinking Calculus 2

As a prerequisite for understanding interpolation, which is key to Numerical Analysis, you must be able to solve the following kind of problem from Calculus 2:

> Suppose we approximate $y = e^x$ on the interval $[0, 1]$ using a Taylor polynomial centered at $x = 0$. How large must the degree of the polynomial be in order to ensure that the absolute error does not exceed 10^{-4}?

Unfortunately, most students in Math 110 find this problem impossible in the beginning, regardless of their Math 53 experience. Now you may have your own theory as to why this may be acceptable. Perhaps you never used Taylor polynomials outside of Calculus, so you forgot about them. Or, perhaps, your Calculus 2 experience was rough and you never understood Taylor stuff in the first place. Be this as it may, you must be able to solve the problem and by 'solve' I mean *understand*. Getting a largely meaningless answer through mimicry is not going to cut it.

Forgetting elementary Calculus is a common and utterly depressing problem in advanced math classes. The common cure for it is the dreaded "calculus review" which we are not going to do. I am willing to bet that you have had your share of reviewing. And still you forget things, so reviewing obviously does not work in the long run. What you need to do is to *rethink* Calculus. This means three things: changing priorities, establishing connections, and distilling the essence.

When you studied Calculus you probably did not have a clear motivation for, say, Taylor theory. You did not think it was important and this was further confirmed outside of Calculus. As a result, your mind did not attach much significance to the topic and, consequently, it quickly slipped out of memory. If you continue to undervalue Taylor theory you will never understand Numerical Analysis. So change its priority to the highest possible level. After all, it is one of the most useful pieces of mathematics that you can learn as an undergraduate.

Now let us talk about connections. Human memory is, as you may know, highly associative. We remember things by establishing physical links in our brains. The more connections, the better we remember things. Conversely, it is hard to remember something if that something does not associate with anything else. You cannot and should not memorize Taylor's theorem on its own. It needs to be associated—connected to other theorems.

Finally, let me try to explain what I mean by distilling the essence. In one of the many Buddhist temples in Kyoto there is a famous painting of six persimmons dating to 13th century; it is displayed to the general public only during major holidays. The painting is just a few quick brush strokes, yet it is cherished by Buddhists and art experts alike. Muqi Fachang—the monk who created that painting—somehow managed to capture the *essence* of six persimmons lying on a table—something that countless imitations and high resolution digital photographs fail to do. This is how you should remember mathematics: in its simplest, most elemental form. In particular, in order to remember Taylor's theorem you need to see the essence of Taylor's theorem. Can you paint it with a few brush strokes?

Figure 1: *Six persimmons*, by Muqi Fachang, ink on paper, 14.25 × 15 in, 13-th century

Value theorems

I hope that after reading the introductory paragraph you have reclassified Taylor's theorem as top priority. If so, let us work on establishing connections between Taylor's theorem and the more basic theorems of analysis. One of those theorems is the Fundamental Theorem of Calculus (FTC) which, I trust, you remember. You can use FTC and integration by parts to derive the Taylor remainder in integral form. However, in order to convert the remainder to the more useful Lagrange form, you need a generalization of the Mean Value Theorem (MVT) which in turn requires Intermediate Value Theorem (IVT) and Extreme Value Theorem (EVT). So we should talk about all three "value" theorems starting with IVT and EVT.

Theorem 1 (IVT). *Let $f \in C[a,b]$. For any $\eta \in [f(a), f(b)]$ there exists $\xi \in [a,b]$ such that $f(\xi) = \eta$.*

We are not going to prove IVT at this point. Instead, let us talk about what it means, why it is nontrivial, and how to remember it. By the way, did you find the format in which I presented IVT [slightly] off-putting? I chose the formal presentation intentionally because it gives us an opportunity to practice active learning. Numerical Analysis, and mathematics in general, is replete with statements such as the one above. You need to learn to decipher mathematical code.

Let us start with the first sentence: "Let $f \in C[a,b]$." This is code for: "Let f be a continuous function defined on a closed interval $[a,b]$." Note that the letter C denotes a *class* of functions—continuous functions; the symbol $\in$ means 'belongs to' or 'element of a set.' Notice also how much more concise the formal statement is compared to its expanded version.

The next sentence asserts the existence of a number ξ in $[a,b]$ such that $f(\xi) = \eta$ as long as the number η lies in the interval $[f(a), f(b)]$. What we are trying to say, using strange Greek letters, is that all of the values between $f(a)$ and $f(b)$ are in the range of f—the function assumes all of these values somewhere in $[a,b]$. So, why not say that? There are several reasons which necessitate Greek letters and other obscurities. One reason is precision. Mathematical statements must be absolutely precise. Common language, on the other hand, is often imprecise and ambiguous. Consider how ambiguous the following statement is (from the mathematical point of view): "Six monks painted six persimmons." Did each monk paint six persimmons? Or did they paint one persimmon each? Another reason for formalism—not always the best one—is brevity. Notice again how much shorter the formal version is compared to the "human" version. I will not use brevity as a pretext for speaking in mathematical code and I will try to avoid being completely formal. Yet, on occasion, we will need to confront formal statements. So, practice!

Now why is IVT nontrivial? Does it not state the obvious? *Intuitively* it does. Consider, however, the formal definition of continuity. In Calculus, the function f is defined to be continuous at ξ if the limit equals the value: $\lim_{x\to\xi} f(x) = f(\xi)$. Try to come up with a formal proof of IVT using the Calculus definition of continuity. Not so trivial now! In fact, IVT is not trivial at all. Its essence has to do with the topology of the real line which we may discuss at some point. In the meantime, try to capture the essence of IVT in a few brush strokes. A deep meditation might help.

Theorem 2 (EVT). *On a closed interval a continuous function assumes its maximum and minimum values.*

The statement is devoid of strange symbolism and does not need to be decoded. Yet, again, it somehow seems trite. Do not maxima and minima always exist? In Calculus I they do and way too much attention is devoted to the mechanical process of finding and testing critical points. In order to appreciate EVT, abstract from the Calculus process for finding extrema. EVT tells you that two things can potentially go wrong when you optimize functions: there may be a discontinuity or the domain may not be closed. For instance, consider $y = x^2$ on $(0, 1]$. This function does not have a minimum because the interval is not closed. No matter which value in $(0, 1]$ is chosen, one can move closer to zero which reduces the value of the function.

Theorem 3 (MVT). *Let $f \in C[a, b]$. There exists $\xi \in [a, b]$ such that:*

$$\int_a^b f(x)\,dx = f(\xi)\,(b-a).$$

This is one way to state the Mean Value Theorem—in *integral form.* Equivalently, we can use FTC to rewrite the above equation as

$$\frac{F(b) - F(a)}{b - a} = F'(\xi).$$

This is the same MVT but stated in differential form. However, the most useful version of MVT (from the point of view of Numerical Analysis) is the one involving a weight. We will call that Generalized Mean Value Theorem (GMVT).

Theorem 4 (GMVT)**.** *Let $f \in C[a,b]$ and suppose that w is a function that maintains constant sign on $[a,b]$. There exists $\xi \in [a,b]$ such that:*

$$\int_a^b f(x)\,w(x)\,dx = f(\xi) \int_a^b w(x)\,dx.$$

Proof. For definitiveness, assume that w is positive. The case where w is negative is completely analogous.

Since f is continuous, it attains its maximum M and its minimum m on $[a,b]$ by EVT. Therefore we have the double inequality:

$$\int_a^b m\,w(x)\,dx \le \int_a^b f(x)\,w(x)\,dx \le \int_a^b M\,w(x)\,dx.$$

Consequently,

$$m \le \frac{\int_a^b f(x)\,w(x)\,dx}{\int_a^b w(x)\,dx} \le M.$$

Now IVT implies that there exists $\xi \in [a,b]$ such that

$$\frac{\int_a^b f(x)\,w(x)\,dx}{\int_a^b w(x)\,dx} = f(\xi).$$

This proves the theorem. ◻

As you will see in the next section, GMVT is very useful for converting error estimates from integral form into simpler derivative form. Indeed, we will often use GMVT for that purpose. In contrast, IVT and EVT are rarely used directly. Nevertheless do not discard EVT and IVT. Doing that ruins the integrity of Calculus which leads to disassociation and memory loss!

We conclude this section with a few remarks about the weight in GMVT. We do not mention it in the statement of the theorem, yet it is implicit that w should be *integrable* on $[a,b]$. What that means is a subject of a long conversation. For now, think of integrability as a condition that rules out "bad" singularities like $\frac{1}{x}$. We hasten to add that unlike f the weight w is not required to be continuous. For example, w can have a jump discontinuity as long as it maintains constant sign. Finally, speaking of the constant sign, that assumption can be somewhat relaxed. For instance, it is OK if w is zero somewhere or even everywhere inside $[a,b]$. What we cannot allow is for w to change sign. Think about the things that go wrong in the proof of GMVT if that happens.

Taylor's theorem

We are ready to discuss Taylor's theorem which we now view as a statement about polynomial interpolation. Quite generally, an interpolating polynomial matches—interpolates—the behavior of the function in some way. Taylor polynomials match the values of the first several derivatives of the function at the center of expansion. In the statement of the theorem we use the symbol C^{n+1} to indicate that a function can be differentiated $(n+1)$ times. This symbol also means that the last $(n+1)$-st derivative is continuous.

Theorem 5 (Taylor)**.** *Let $f \in C^{n+1}[a,b]$. Then for any x and $x_0 \in (a,b)$*

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!}\,(x-x_0)^k + \frac{f^{(n+1)}(\xi)}{(n+1)!}\,(x-x_0)^{n+1},$$

where ξ lies between x_0 and x.

Proof. Using FTC, we can write

$$f(x) = f(x_0) + \int_{x_0}^{x} f'(t)\,dt.$$

This is a special form of Taylor's theorem valid if $f \in C^1[a,b]$. If $f \in C^2[a,b]$ we can use integration by parts to rewrite the above equation as:

$$f(x) = f(x_0) + f'(x_0)\,(x-x_0) + \int_{x_0}^{x} (x-t)\,f''(t)\,dt.$$

For $f \in C^{n+1}[a,b]$ repeated integration by parts leads to

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!}\,(x-x_0)^k + \int_{x_0}^{x} \frac{(x-t)^n}{n!}\,f^{(n+1)}(t)\,dt.$$

This is Taylor's theorem but with remainder in integral form. To finish the proof we apply GMVT. Since $f \in C^{n+1}$ the derivative $f^{(n+1)}$ is continuous. Furthermore, the weight $w(t) = (x-t)^n/n!$ is of constant sign on $[x_0, x]$. Hence

$$\begin{aligned}\int_{x_0}^{x} \frac{(x-t)^n}{n!}\,f^{(n+1)}(t)\,dt &= f^{(n+1)}(\xi)\,\int_{x_0}^{x} \frac{(x-t)^n}{n!}\,dt \\ &= f^{(n+1)}(\xi)\,\frac{(x-x_0)^{n+1}}{(n+1)!}.\end{aligned}$$

This completes the proof. □

Let us return to the problem about approximating e^x on $[0, 1]$ with Taylor polynomials centered at zero. For the exponential, the Taylor polynomial of degree n at the origin is given by

$$T_n = \sum_{k=0}^{n} \frac{x^k}{k!}.$$

According to Taylor's theorem, the absolute error of n-th degree approximation is

$$|e^x - T_n(x)| = e^{\xi} \, \frac{|x|^{n+1}}{(n+1)!}$$

with $\xi \in [0, x]$. Since e^x is monotonely increasing, the worst possible case is when $x = \xi = 1$. Thus the error is bounded by $1/(n + 1)!$ and we need to choose n so that

$$\frac{1}{(n+1)!} < 10^{-4}.$$

This requires $n \geq 7$.

Lagrange interpolation

A Taylor polynomial matches, or interpolates, the values of several derivatives of a function at a single point. In contrast, the Lagrange polynomial interpolates the values of a function at several distinct points which we will call *nodes*.

Thus the Lagrange polynomial p interpolating f at nodes $x_1, \ldots, x_n$ is the polynomial satisfying

$$p(x_k) = f(x_k), \quad \text{for } k = 1, \ldots, n.$$

The degree of such a polynomial must necessarily be $(n - 1)$. In the special case of two nodes the Lagrange polynomial is just the familiar secant line:

$$p = \frac{f(x_2) - f(x_1)}{x_2 - x_1} \, (x - x_1) + f(x_1)$$

Lagrange polynomials of higher degree are a bit more complicated and will be discussed later. In the meantime, suppose we interpolate f at two distinct nodes. What is the error of interpolation?

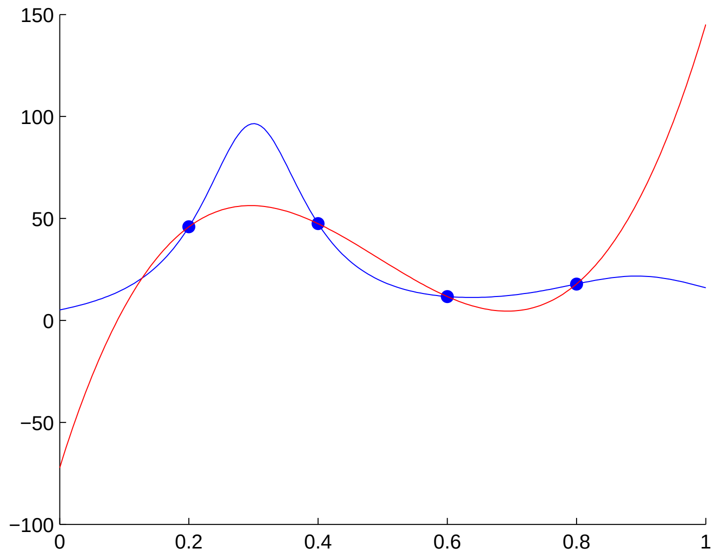

Figure 2: Lagrange cubic (red) interpolating `humps` (blue) at four equispaced nodes in $[0,1]$

Remainder of linear interpolation

For notational convenience let us label the two nodes a and b ($b > a$) and let

$$R(x) = f(x) - p(x) = f(x) - f(a) - \frac{f(b) - f(a)}{b - a}(x - a).$$

This is the remainder of linear Lagrange interpolation. If we let b approach a we should get the remainder for (linear) Taylor interpolation. This suggests that there should be some similarity with Taylor theory. In particular, we should expect the second derivative to be involved and therefore we should assume that $f \in C^2$.

In order to find an expression for R, we first observe that it satisfies the following boundary value problem:

$$R'' = f'', \quad R(a) = R(b) = 0.$$

Boundary value problems are usually more difficult than initial value problems which you studied in Math 57. However in this particular case the solution can be derived using simple calculus as follows. Integrate the differential equation twice using a as the lower limit. This gives:

$$R = \int_a^x \left[\int_a^s f''(t)\, dt \right] ds + C_1 + C_2\, x.$$

From boundary conditions we infer that

$$\begin{aligned} C_1 + C_2\, a &= 0 \\ C_1 + C_2\, b &= -\int_a^b \left[\int_a^s f''(t)\, dt \right] ds \end{aligned}$$

Therefore

$$R = \int_a^x \left[\int_a^s f''(t)\, dt \right] ds - \frac{(x-a)}{b-a} \int_a^b \left[\int_a^s f''(t)\, dt \right] ds.$$

We now reverse the order of integration (as you did in Math 55) which gives:

$$R = \int_a^x (x-t)\, f''(t)\, dt - \frac{(x-a)}{b-a} \int_a^b (b-t)\, f''(t)\, dt$$

This can be put in the form

$$R = \int_a^b K(x,t)\, f''(t)\, dt$$

where the *kernel* K is given by:

$$K(x,t) = -\frac{1}{b-a} \begin{cases} (t-a)\,(b-x), & a < t \leq x, \\ (x-a)\,(b-t), & x < t < b. \end{cases}$$

We have thus succeed in expressing the remainder of Lagrange interpolation as an integral. If you followed the discussion of Taylor's remainder then you know that the next step is to apply GMVT. Since $a \leq x \leq b$ the kernel K maintains constant (negative) sign on $[a,b]$ (sketch it!). Therefore, by GMVT:

$$R = f''(\xi) \int_a^b K(x,t)\, dt = \frac{1}{2} f''(\xi)(x-a)\,(x-b).$$

Notice that we recover Taylor's remainder if $b \to a$.

Remainder for Lagrange interpolation

Following the discussion of linear interpolation, it is easy to guess the general statement which we prove below.

Theorem 6 (Lagrange)**.** *Let $f \in C^n[a,b]$ and let p denote the interpolating polynomial with nodes $\{x_1, \ldots, x_n\}$. The remainder of interpolation is*

$$f(x) - p(x) = \frac{f^{(n)}(\xi)}{n!}\,(x - x_1)\,(x - x_2)\ldots(x - x_n).$$

Proof. Let

$$w(t) = \prod_{k=1}^{n}(t - x_k)$$

be the *nodal polynomial.* Fix x and introduce the following auxiliary function (of t):

$$g(t) = f(t) - p(t) - (f(x) - p(x))\,\frac{w(t)}{w(x)}.$$

The function g is C^n (since f is). Also, since $f(x_k) = p(x_k)$ and $w(x_k) = 0$ we have

$$g(x_k) = 0, \quad k = 1, \ldots, n.$$

Moreover, $g(x) = 0$, by construction. Thus g has $n+1$ zeros. It now follows from generalized Rolle's theorem that there is a ξ such that $g^{(n)}(\xi) = 0$. If you do not know [generalized] Rolle's theorem, recall MVT in differential form:

$$\frac{F(b) - F(a)}{b - a} = F'(\xi).$$

If $F(b) = F(a) = 0$ then $F'(\xi) = 0$: the derivative of a function with two zeros must vanish somewhere. If a function has three zeros, its first derivative has at least two zeros, so the second derivative must vanish somewhere. Generalized Rolle's theorem is simply induction of MVT: if a C^n function has $(n+1)$ zeros then its n-th derivative must vanish somewhere. Now the n-th derivative of the cleverly constructed g is:

$$g^{(n)}(\xi) = f^{(n)}(\xi) - (f(x) - p(x))\,\frac{n!}{w(x)}.$$

Setting this expression to zero and solving for $f(x) - p(x)$ gives the statement of the theorem.

$\square$

The proof of Theorem 6 is, objectively, sleek and requires seemingly less effort compared to solving a boundary value problem. However it is not constructive. One has to know what the remainder is and, further, have the ingenuity to come up with a useful auxiliary function. A lot of proofs in textbooks are sleek but not constructive. This is why few non-mathematicians bother to read mathematical textbooks.

Exercises

1. Derive the remainder of Lagrange interpolation for three nodes by solving an appropriate boundary value problem. Show that the formula is consistent with Taylor theory.

2. In `Matlab` one can find Lagrange polynomials using `polyfit` command. Write a script that plots Lagrange polynomials through N equispaced nodes $\{x_k = k/(N+1)\}$, $k = 1, ..., N$ for $f(x) = e^x$. What happens as N increases?

3. Repeat the previous exercise with `Matlab`'s `humps` function in place of the exponential. What are your observations?