Math 128A, Summer 2019
Lecture 13, Monday 7/15/2019

CLASS ANNOUNCEMENTS: Midterm on Wednesday, only 1 hour long, 3 problems. No (numerical) integration.
Goals today: Talk about Numerical integration, also known as Quadrature.

1 Homework 4 Review

1.1 Problem 1

Recall problem 1 asks us to interpolate

$$f(t) = \frac{1}{1+t^6}.$$

Consider the system of linear equations

$$\sum_{j=0}^{n}$$

In the solution I already built, we demonstrated that interpolation in the monomial basis is bad (θ^k). Consider instead:

1.2 Error in Hermite Interpolation

$$f(t) - p(t) = \frac{f^{(2n+2)}(\xi)}{(2n+2)!}\left[\omega(t)\right]^2$$

We say that the error is bounded by $f^{(2n+2)}(\xi)$, which we (optionally, in 128B) express in norms:

$$\|f\|_\infty = \max_x |f(x)|.$$

2 Quadrature (Numerical Integration)

We call numerical integration sometimes as quadrature because in the old days, we would draw grids and count the squares for the 'area under the curve' for integration.
Today we'll talk about the **Trapezoidal rule**, **not to derive Newton-Cotes** as it is bad, but rather talk about **Endpoint correction**. That is, we look at two things: δ_{jk}^m and the Euler-Maclaurin summation formula.
The general idea of numerical integration:

$$\int_a^b f(x)\ dx = \int_a^b p(x)\ dx + \int_a^b E(x)\ dx,$$

where $p(x)$ is an approximating polynomial (something we know how to approximate), and $E(x)$ is the error.

For example, $p(x)$ interpolates $f(x)$ at $x_0, \ldots, x_n$. This implies $p(x_j) = f(x_j)$ for $0 \leq j \leq n$.

$$\begin{aligned}
\int_a^b p(x)\ dx &= \int_a^b f(x_0)L_0(x) + \cdots + f(x_n)L_n(x)\ dx \\
&= f(x_0)\underbrace{\int_a^b L_0(x)\ dx}_{w_0} + \cdots + f(x_n)\underbrace{\int_a^b L_n(x)\ dx}_{w_n} \\
&= w_0 f(x_0) + w_1 f(x_1) + \cdots + w_n f(x_n)
\end{aligned}$$

So we take the Lagrange-basis . This is a once-in-a-lifetime calculation, as they do not depend on f. We call these the weights $w_0, \ldots, w_n$.
Let's look at the stupidest possible example:

$$\begin{aligned}
n = 0: \qquad p(x) &= f(x_0) \cdot 1 \\
L_0(x) &= 1 \\
\int_a^b L_0(x)\ dx &= b - a =: w_0
\end{aligned}$$

Hence:

$$\int_a^b f(x)\ dx \approx (b-a)f(x_0).$$

Then for our error, we can write:

$$\int_a^b f(x)\ dx - [w_0 f(x_0) + \cdots + w_n f(x_n)] = \int_a^b \frac{f^{(n+1)}(\xi(x))}{(n+1)!}\omega(x)\ dx$$

This is not a particularly useful error formula
If $\omega(x)$ **does not change sign** over our interval $[a, b]$, then we can use the MVT for integrals to estimate:

$$\text{error} = \frac{f^{(n+1)}(\varphi)}{(n+1)!}\int_a^b \omega(x)\ dx,$$

where $\varphi \in [a, b]$ is some unknown point.
Otherwise, we have:

$$\begin{aligned}
|\text{error}| &\leq \int_a^b \frac{|f^{(n+1)}(\xi(x))|}{(n+1)!}|\omega(x)|\ dx \\
&\leq \frac{\max_x |f^{(n+1)}(x)|}{(n+1)!}\underbrace{\int_a^b |\omega(x)|}_{\text{constant}}\ dx
\end{aligned}$$

where the second inequality follows directly from the triangle inequality.

Example : $n = 1$:

$$p(x) = \underbrace{\frac{x - x_1}{x_0 - x_1}}_{L_0(x)} f(x_0) + \underbrace{\frac{x - x_0}{x_1 - x_0}}_{L_1(x)} f(x_1)$$

Solution. Consider:

$$\int_a^b \frac{x - x_1}{x_0 - x_1}\ dx = \frac{1}{2}\frac{(b - x_1)^2 - (a - x_1)^2}{x_0 - x_1}$$

Then this gives:

$$\int_a^b f(x)\ dx = f(x_0)w_0 + f(x_1)w_1$$

We'll use the Trapezoidal Rule, in that if $x_0 := a$ and $x_1 := b$, the above gives:

$$w_0 = \frac{1}{2}\frac{-(a-b)^2}{a-b} = \frac{1}{2}(b-a) > 0 \text{if } b > a.$$

And we get w_1 for free; that is:

$$w_1 = \underbrace{w_0 + w_1}_{\approx \int_a^b 1\ dx} + w_0$$

And this is a constant integral, so we conclude:

$$\begin{aligned} &w_0 + w_1 = w_0 \cdot 1 + w_1 \cdot 1 = \int_a^b 1\ dx = (b-a) \\ &\implies w_1 = \frac{1}{2}(b-a) \end{aligned}$$

Usually we start off Trapezoidal Rule by writing:

$$\int_a^b f(t)\ dt = \frac{1}{2}f(0) + \frac{1}{2}f(1) + E,$$

where

$$\begin{aligned} E &= \int_0^1 \frac{f''(\xi)}{2!}(t-0)(t-1)\ dt \\ &= \frac{f''(\xi)}{2!}\int_0^1 (t)(t-1)\ dt \\ &= \frac{1}{2!}\cdot\left(\frac{1}{3} - \frac{1}{2}\right) f''(\xi) \\ &= \frac{-1}{12} f''(\xi) \end{aligned}$$

$\square$

2.1 Compounding

We take the interval $[a, b]$ and break down into intervals:

$$\begin{aligned} [a,b] &= [a, a+h] \cup [a+h, a+2h] \cup \cdots \cup [b-h, b], \qquad h = \frac{b-a}{n} \\ &= \bigcup_{j=0}^{n-1} [a + jh, a + (j+1)h] \end{aligned}$$

and we get:

$$\int_a^b f(x)\ dx = \sum_{j=0}^{n-1}\left[\underbrace{\int_{a+jh}^{a+(j+1)h} f(x)\ dx}\right]$$

Runge says to not interpolate a function and use the entirety of the interval to perform integration with one high-degree interval and calculating weights across the entire interval. Instead, we 'derive' the obvious Trapezoidal Rule simply taking the linear interpolants of each small interval.
That is, for our previous example we have:

$$\begin{aligned}\int_a^b f(x)\ dx &= \sum_{j=0}^{n-1}\left[\underbrace{\int_{a+jh}^{a+(j+1)h} f(x)\ dx}\right]\\ &= \frac{1}{2}hf(a+jh)+\frac{1}{2}hf(a+(j+1)h),\end{aligned}$$

and

$$E = \frac{-h^3}{12}f''(\xi),$$

where the power of 3 follows from the dimension of $1 \to h$ changing

$$\frac{1}{2}f(0)+\frac{}{2}f(1)+E \to \frac{1}{2}f(0)+\frac{}{2}f(1)+E;$$

and hence our error E has dimensions

$$\frac{HF}{H^2},$$

and in order to compensate, we need to insert $1 \mapsto h^3$ in the error formula in changing from the $[0,1]$ interval to smaller intervals).
So in all, we have:

$$\begin{aligned}\int_a^b f(x)\ dx &= \sum_{j=0}^{n-1}\underbrace{\frac{1}{2}hf_j+\frac{1}{2}hf_{j+1}}-\frac{1}{12}\sum_{j=0}^{n-1}h^3f''(\xi_j)\\ &\quad \frac{1}{2}h\left(\underbrace{f_0+f_1}+\underbrace{f_1+f_2}+\cdots\right)\\ &= h\left(\frac{1}{2}f_0+f_1+\cdots+f_{n-1}+\frac{1}{2}f_n\right) \quad \text{Trapezoidal Rule}\\ &\quad -\frac{h^3}{12}f''(\xi) \quad \text{Error term}\end{aligned}$$

Whatever oscillation we have can be blamed entirely on f and not our integration formula / algorithm, unlike in Newton-Cotes.
Define $f_j := f(a+jh)$. In summary, our Compound Trapezoidal Rule gives us:

$$\int_a^b f(x)\ dx = h\underbrace{\sum_{j=0}^{n} f_j}-\frac{h^2}{12}\frac{b-a}{n}\sum_{j=0}^{n-1}f''(\xi_j),$$

where the underbraced term is equal to $\frac{1}{2}$ on the first and last terms, and our sum on the right is an average (MVT). So we write:

$$\int_a^b f(x)\ dx = h\sum_{j=0}^{n} -\frac{h^2}{12}(b-a)f''(\xi)$$

The rate of convergence is $O(h^2) = O(\frac{1}{n^2}) = \varepsilon$. We say that the work required is

$$n = O(\varepsilon^{-1/2}) = O\left(\frac{1}{\sqrt{\varepsilon}}\right)$$

It turns out that this is quite pessimistic.

3 Deriving the Euler-Maclaurin Summation Formula

The Euler-Maclaurin Summation Formula tells us **exactly** what the error above is. Recall that earlier in the course, we integrated by parts to obtain:

$$\begin{aligned}
\int_0^1 f(t)\ dt &= \int_0^1 \frac{d}{dt}\ \left(t-\frac{1}{2}\right) f(t)\ dt \\
&= \left(t-\frac{1}{2}\right) f(t)|_0^1 - \int_0^1 \left[\frac{1}{2}\left(t-\frac{1}{2}\right)^2\right]' f'(t)\ dt \\
&= \left(t-\frac{1}{2}\right) f(t)|_0^1 - \frac{1}{2}\left(t-\frac{1}{2}\right)^2 f'(t)|_0^1 + \int_0^1 \left[\frac{1}{3!}\left(t-\frac{1}{2}\right)^3\right]' f''(t)\ dt \\
&= \left(t-\frac{1}{2}\right) f(t) - \frac{1}{2}\left(t-\frac{1}{2}\right)^2 f'(t) + \frac{1}{3!}\left(t-\frac{1}{2}\right)^3 f''(t) - \frac{1}{4!}\left(t-\frac{1}{2}\right)^4 f'''(t) + \cdots\Big|_0^1
\end{aligned}$$

But the factors in parentheses are $\pm\left(\frac{1}{2}\right)^k$ at $t = 0, 1$, acting as averages and differences at the two points on the interval. Numerically evaluating, this gives us:

$$\begin{aligned}
\int_0^1 f(t)\ dt = \frac{1}{1!}\left(\frac{1}{2}\right)^1 &[f(1)+f(0)] \\
&- \frac{1}{2!}\left(\frac{1}{2}\right)^2 [f'(1)-f'(0)] \\
&+ \frac{1}{3!}\left(\frac{1}{2}\right)^3 [f''(1)-f''(0)] \\
&- \frac{1}{4!}\left(\frac{1}{2}\right)^4 [f'''(1)-f'''(0)] + \cdots
\end{aligned}$$

Thus we conclude that the Trapezoidal Rule gives us:

$$\frac{1}{2}[f(1)-f(0)] = \int_0^1 f(t)\ dt + \frac{1}{2!}\left(\frac{1}{2}\right)^2 [f'(1)-f'(0)] - \frac{1}{3!}\left(\frac{1}{2}\right)^3 [f''(1)+f''(0)] - \cdots$$

We get a telescoping (cancelling) series:

$$\begin{aligned}
\left[\sum_{j=0}^{n} f(j)\right] &= \frac{1}{2}\left(f(1)-f(0)\right)+\frac{1}{2}\left(f(2)+f(1)\right)+\cdots+\frac{1}{2}\left(f(n)+f(n-1)\right) \\
&= \int_0^n f(x)\ dx + \frac{1}{2!}\left(\frac{1}{2}\right)^2 [f'(n)-f'(0)] \\
&\quad - \frac{1}{3!}\left(\frac{1}{2}\right)^3 \sum_{j=0}^{n} f''(j) \\
&\quad + \frac{1}{4!}\left(\frac{1}{2}\right)^4 [f'''(n)-f'''(0)] \\
&\quad - \frac{1}{5!}\left(\frac{1}{2}\right)^5 \sum_{j=0}^{n} f'''(j) + \cdots
\end{aligned}$$

We have the actual integral plus some error, where half the error terms are beautiful, and don't look beautiful. So we want some way to 'kill' the even-numbered derivatives.

$$\frac{1}{2}[f(1)-f(0)] = \int_0^1 f(t)\ dt + \frac{1}{2!}\left(\frac{1}{2}\right)^2 \underbrace{[f'(1)-f'(0)]}_{\text{good}} - \frac{1}{3!}\left(\frac{1}{2}\right)^3 \underbrace{[f''(1)+f''(0)]}_{\text{bad}} - \cdots$$

$$\frac{1}{2}\underbrace{[f''(1)-f''(0)]}_{\text{bad}} = \int_0^1 f''(t)\ dt + \frac{1}{2!}\left(\frac{1}{2}\right)^2 [f'''(1)-f'''(0)] - \frac{1}{3!}\left(\frac{1}{2}\right)^3 [f''''(1)+f''''(0)] - \cdots$$

But notice

$$\sum_0^1 f''(t)\ dt = f'(1)-f'(0).$$

So we have:

$$\begin{aligned}
\int_0^1 f(t)\ dt &= \frac{1}{2}[f(1)+f(0)] \\
&\quad + b_1 [f'(1)-f'(0)] \\
&\quad + b_2 \left[f^{(3)}(1)-f^{(3)}(0)\right] \\
&\quad + b_3 \left[f^{(5)}(1)-f^{(5)}(0)\right] \\
&\quad + \cdots
\end{aligned}$$

And we conclude the **Euler-Maclaurin Summation Formula**:

$$\int_0^n f(x)\ dx = \sum_{j=0}^{n} f(j) + b_1 [f'(n)-f'(0)] + b_2 \left[f^{(3)}(n)-f^{(3)}(0)\right] + \cdots$$

Remark: The idea is that no matter how long our integration interval is, the **error** from the Trapezoidal Rule only depends on the **endpoints**.

To kill the 'bad' averaging terms, because f is an arbitrary function, we 'plug in' f'' (double-prime), and we saw that we pushed the bad terms back by two.

Remark: Intuitively, because our error only depends on the endpoints, we can change the weights at the ends to be less (like $\frac{3h}{8}, \frac{5h}{8}, h, \ldots, h\frac{5h}{8}, \frac{3h}{8}$). More about this via 'Endpoint Correction'.

Lecture ends here.

We can see this neatly in Strain's handout on ECTR (Endpoint Corrections, Trapezoidal Rule).

Euler-Maclaurin formula Integrate by parts as in Taylor expansion:

$$\begin{aligned}
& \int_0^1 f(x)dx = \int_0^1 \frac{d}{dx}(x-1/2)f(x)dx \\
= \; & (1/2)(f(0)+f(1)) - \int_0^1 (x-1/2)f'(x)dx \\
= \; & (1/2)(f(0)+f(1)) - \int_0^1 \frac{d}{dx}\frac{1}{2}(x-1/2)^2 f'(x)dx \\
= \; & (1/2)(f(0)+f(1)) - \frac{1}{2}(1/2)^2(f'(1)-f'(0)) + \int_0^1 \frac{d}{dx}\frac{1}{3!}(x-1/2)^3 f''(x)dx \\
= \; & (1/2)(f(0)+f(1)) - \frac{1}{2!}(1/2)^2(f'(1)-f'(0)) + \frac{1}{3!}(1/2)^3(f''(1)+f''(0)) - \int_0^1 \frac{d}{dx}\frac{1}{4!}(x-1/2)^4 f'''(x)dx
\end{aligned}$$

and so forth. Rearrange to get an error formula for the trapezoidal rule:

$$(1/2)(f(0)+f(1)) = \int_0^1 f(x)dx + \frac{1}{2!}(1/2)^2(f'(1)-f'(0)) - \frac{1}{3!}(1/2)^3(f''(1)+f''(0)) + \int_0^1 \frac{d}{dx}\frac{1}{4!}(x-1/2)^4 f'''(x)dx.$$

Apply the formula to f'' in place of f:

$$\begin{aligned}
& (1/2)(f''(0)+f''(1)) = \int_0^1 f''(x)dx + \frac{1}{2!}(1/2)^2(f'''(1)-f'''(0)) - \frac{1}{3!}(1/2)^3(f''''(1)+f''''(0)) + \cdots \\
= \; & f'(1)-f'(0) + \frac{1}{2!}(1/2)^2(f'''(1)-f'''(0)) - \frac{1}{3!}(1/2)^3(f''''(1)+f''''(0)) + \int_0^1 \frac{d}{dx}\frac{1}{4!}(x-1/2)^4 f'''''(x)dx.
\end{aligned}$$

Key step: Use the result to eliminate the term involving $f''(1)+f''(0)$ from the previous formula:

$$(1/2)(f(0)+f(1)) = \int_0^1 f(x)dx + (1/12)(f'(1)-f'(0)) + \frac{1}{2!}(1/2)^2(f'''(1)-f'''(0)) + \int_0^1 \frac{d}{dx}\frac{1}{4!}(x-1/2)^4 f'''(x)dx.$$

Now imagine repeating the elimination infinitely often. The result would be to eliminate all the terms with plus signs between even derivatives of f and leave an infinite series of the form

$$(1/2)(f(0)+f(1)) = \int_0^1 f(x)dx + b_1(f'(1)-f'(0)) + b_2(f'''(1)-f'''(0)) + b_3(f'''''(1)-f'''''(0)) + \cdots$$

with some unknown constants $b_1 = 1/12$, b_2, b_3, ..., multiplying differences of odd-numbered derivatives of f. The Euler-Maclaurin summation formula follows by compounding:

$$\frac{1}{2}f(0) + f(1) + f(2) + \cdots + f(n-1) + \frac{1}{2}f(n) = \int_0^n f(x)dx + b_1(f'(n)-f'(0)) + b_2(f'''(n)-f'''(0)) + \cdots$$

because the differences of derivatives all telescope, canceling the interior terms. Conclusion: The error in the trapezoidal rule depends only on the derivatives of the integrand at the endpoints of the domain of integration. For example, the trapezoidal rule integrates a smooth periodic function over a full period with great accuracy.

ECTR It follows that the order of accuracy (degree of precision) of the trapezoidal rule can be increased by *endpoint corrections* which change the weights only near the endpoints of the interval. Such corrections can be derived by coupling the Euler-Maclaurin formula with finite difference approximations to the derivatives, or by polynomial interpolation as follows.

Let's use cubic interpolation to derive a fourth-order endpoint corrected trapezoidal rule. To do this, we interpolate four successive function values f_0, f_1, f_2, f_3 to integrate over the interval $[1, 2]$. Since the Lagrange basis functions are

$$L_0(x) = (x-1)(x-2)(x-3)/(0-1)(0-2)(0-3) = (x-1)(x-2)(x-3)/(-6)$$

$$L_0(x) = (x-1)(x-2)(x-3)/(0-1)(0-2)(0-3) = (x-1)(x-2)(x-3)/(-6)$$

$$\begin{aligned}
L_1(x) &= (x-0)(x-2)(x-3)/(1-0)(1-2)(1-3) = (x-0)(x-2)(x-3)/2 \\
L_2(x) &= (x-0)(x-1)(x-3)/(2-0)(2-1)(2-3) = (x-0)(x-1)(x-3)/(-2) \\
L_3(x) &= (x-0)(x-1)(x-2)/(3-0)(3-1)(3-2) = (x-0)(x-1)(x-2)/6
\end{aligned}$$

the resulting rule is

$$\int_1^2 f(x)dx = w_0 f(0) + w_1 f(1) + w_2 f(2) + w_3 f(3)$$

where

$$w_0 = \int_1^2 L_0(x)dx = -1/24 = w_3$$

and

$$w_1 = \int_1^2 L_1(x)dx = 13/24 = w_2.$$

At the end intervals such as $[0,1]$ we do not have $f(-1)$ so we drop to quadratic interpolation with

$$L_0(x) = (x-1)(x-2)/(0-1)(0-2) = (x-1)(x-2)/2$$

$$\begin{aligned}
L_1(x) &= (x-0)(x-2)/(1-0)(1-2) = (x-0)(x-2)/(-1) \\
L_2(x) &= (x-0)(x-1)/(2-0)(2-1) = (x-0)(x-1)/2
\end{aligned}$$

The resulting rule is

$$\int_0^1 f(x)dx = w_0 f(0) + w_1 f(1) + w_2 f(2)$$

where

$$w_0 = 10/24, \qquad w_1 = 16/24, \qquad w_2 = -2/24.$$

Putting it all together gives the fourth-order endpoint corrected trapezoidal rule

$$\int_0^1 f(x)dx = \frac{h}{24}\left(9f(0) + 23f(h) + 28f(2h) + 24f(3h) + 24f(4h) + \cdots + 9f(nh)\right).$$