MAT 128A - Assignment 8

Karry Wong

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Problem 1

Let $x_0 = 0, x_1 = \frac{1}{2}, x_2 = 1$. Find weights w_0, w_1, and w_2 such that the formula

$$\int_0^1 f(x)\,dx = w_0 f(x_0) + w_1 f(x_1) + w_2 f(x_2) \tag{1}$$

holds whenever f is a polynomial of degree less than or equal to 2.

Ans: Same as Simpson's rule (the closed Newton-Cotes formula for three points) shown in lecture 18, we substitute

$$f_1(x) = 1, \quad f_2(x) = x, \quad f_3(x) = x^2$$

into (1). We obtain

$$\begin{cases} 1 = \int_0^1 1\,dx & = w_0 \cdot 1 + w_1 \cdot 1 + w_2 \cdot 1 \\ \frac{1}{2} = \int_0^1 x\,dx & = w_0 \cdot 0 + w_1 \cdot \frac{1}{2} + w_2 \cdot 1 \\ \frac{1}{3} = \int_0^1 x^2\,dx & = w_0 \cdot 0 + w_1 \cdot \left(\frac{1}{2}\right)^2 + w_2 \cdot 1^2 \end{cases} \quad \Rightarrow \quad w_0 = \frac{1}{6},\ w_1 = \frac{2}{3},\ w_2 = \frac{1}{6}$$

As shown in class, for arbitrary interval $[a, b]$, the *weights* for Simpson's rule are $w_0 = \frac{b-a}{6}$, $w_1 = \frac{2(b-a)}{3}$, $w_2 = \frac{b-a}{6}$.

Remark 1. Assume that the function f is at least four times continuously differentiable on $[a, b]$ and c is the midpoint of interval $[a, b]$, i.e. $c = \frac{a+b}{2}$. Let $h = c - a = b - c$. Simpson's rule states that there exists a point $\xi \in (a, b)$ such that

$$\int_a^b f(x)dx = \frac{h}{3}[f(a) + 4f(c) + f(b)] - \underbrace{\frac{h^5}{90} f^{(4)}(\xi)}_{\text{error term}}$$

Since the error term involves the fourth derivative of f, Simpson rule is indeed exact for polynomial of degree equal to or less than three!

Bonus I: For those who are interested in learning more, let me first show you how to "cheat" in obtaining the right coefficient for the error term in Simpson's rule:

Let f be a function that is at least four times continuously differentiable on an interval $[a,b]$. Let midpoint of the interval be $c = \frac{a+b}{2}$ and the spacing be $h = c - a = b - c$. Assume that we know the error term is $\mathcal{O}(h^5)$ instead of $\mathcal{O}(h^4)$ involving the fourth derivative of $f(x)$ (**that is a big assumption to make!**), then we have for $\xi \in (a,b)$,

$$\int_a^b f(x)\,dx = \frac{h}{3}[f(a) + 4f(c) + f(b)] + kf^{(4)}(\xi)$$

where k is a constant. In order to solve for k, the key idea is to apply the above formula on $f(x) = x^4$. Together with $c = \frac{a+b}{2}$, $h = \frac{b-a}{2}$, we have

$$\begin{aligned} \int_a^b x^4\,dx &= \frac{b-a}{6}(a^4 + 4c^4 + b^4) + k(24) \quad \text{since } f^{(4)}(x) \equiv 24 \\ \Rightarrow \quad \frac{b^5 - a^5}{5} &= \frac{b-a}{6}(a^4 + \frac{1}{4}(a+b)^4 + b^4) + k(24) \\ \Rightarrow \quad 24k &= \frac{b^5 - a^5}{5} - \frac{b-a}{24}(4a^4 + (a+b)^4 + 4b^4) \end{aligned}$$

If you have lot of time in expanding the RHS of the above equation and calculate carefully (or simply use `Mathematica`), you will arrive at

$$24k = \frac{1}{120}(a-b)^5 \quad \Rightarrow \quad k = -\frac{1}{2880}(b-a)^5 \quad \Rightarrow \quad k = -\frac{h^5}{90}$$

Bonus II: At the end of the lecture 18, Prof. Bremer mentioned the error estimate for Simpson rule, i.e. how to derive the term $-\frac{h^5}{90}f^{(4)}(\xi)$. The main idea is to integrate the error term obtained from the Lagrange interpolation formula. **Unfortunately, unlike the error estimate in the trapezoidal rule, we cannot apply the weighted mean value theorem directly due to change of sign in the cubic polynomial inside the integrand.** Let me show you here how to get around it ☺

Let f be a function that is at least four times continuously differentiable on an interval $[a,b]$. Let midpoint of the interval be $c = \frac{a+b}{2}$ and the spacing be $h = c - a = b - c$. The error term is the integral of the Lagrange interpolation error, i.e.

$$Err := \int_a^b \frac{f^{(3)}(\xi(x))}{3!}(x-a)(x-c)(x-b)\,dx, \qquad \text{where } \xi(x) \text{is a function of x!}$$

For those of you who know about *divided difference*, indeed $\frac{f^{(3)}(\xi(x))}{3!} = f[a,b,c,x]$.

the key idea here is to use integration by parts, first define $w(x) := \int_a^x (t-a)(t-c)(t-b)\,dt$.

Notice that $w'(x) = (x-a)(x-c)(x-b)$ follows immediately. Also, clearly $w(a) = 0$.

Since the cubic polynomial $g(t) \coloneqq (t-a)(t-c)(t-b)$ is "rotational symmetric" around $t = c$, i.e. $g(-t+2c) = -g(t)$, and a, c, b are equally spaced, so $w(b) = 0$. (Draw a picture or compute the integral explicitly!).

Lastly, $w'(x) = (x-a)(x-c)(x-b) > 0$ for $a < x < c$ and $w'(x) = (x-a)(x-c)(x-b) < 0$ for $c < x < b$, so $w'(x)$ attains local maximum at $x = c$. Combining all the above information, we know that $w(x) > 0$ for all $x \in (a,b)$, i.e. $w(x)$ **does not change sign**.

$$
\begin{aligned}
Err &= \int_a^b f[a,b,c,x]w'(x)\,dx = \underbrace{\Big[f[a,b,c,x]w(x) \Big]_a^b}_{=0-0=0} - \int_a^b \frac{d}{dx}\left(f[a,b,c,x]\right) w(x)\,dx \\
&\overset{(\diamond)}{=} -\int_a^b f[a,b,c,x,x]w(x)\,dx \overset{(*)}{=} -f[a,b,c,\eta,\eta]\int_a^b w(x)\,dx
\end{aligned}
$$

for some $\eta \in (a,b)$.

$(\diamond)$ holds since divided difference is invariant under permutation, we have

$$
\begin{aligned}
\frac{d}{dx}\left(f[a,b,c,x]\right) &= \lim_{h\to 0}\frac{f[a,b,c,x+h] - f[a,b,c,x]}{h} = \lim_{h\to 0}\frac{f[a,b,c,x+h] - f[x,a,b,c]}{h} \\
&= \lim_{h\to 0} f[x,a,b,c,x+h] = f[x,a,b,c,x] = f[a,b,c,x,x]
\end{aligned}
$$

Important: At $(*)$, the weighted mean value theorem can be applied since $w(x)$ does not change sign.

Now there is a corresponding Mean Value Theorem for divided difference which states that for any $(n+1)$ distinct numbers $x_0, \cdots, x_n$ in $[a,b]$, we have

$$
f[x_0, x_1, \cdots, x_n] = \frac{f^{(n)}(\bar\eta)}{n!} \quad \text{for some } \bar\eta \in \left(\min_i\{x_i\}, \max_i\{x_i\}\right)
$$

Therefore, $Err = -\frac{f^{(4)}(\bar\eta)}{4!}\int_a^b w(x)\,dx$. for some $\bar\eta \in (a,b)$

Finally, we compute $\int_a^b w(x)\,dx$,

$$
\int_a^b w(x)\,dx = \int_a^b \int_a^x (t-a)(t-c)(t-b)\,dt\,dx = \cdots = \frac{4}{15}h^5
$$

It took me some time to evaluate this integral. (Again, using `Mathematica` is always an option!)

Therefore, we have

$$
Err = \int_a^b \frac{f^{(3)}(\xi(x))}{3!}(x-a)(x-c)(x-b)\,dx = -\frac{f^{(4)}(\bar\eta)}{24}\cdot\frac{4}{15}h^5 = -\frac{h^5}{90}f^{(4)}(\bar\eta)
$$

Alternatively, here is a sketch of another idea from Prof. Bremer: Let $p(x)$ be the degree 2 polynomial that interpolates $f(x)$ at a, c, b. We replace the term $\frac{f^{(3)}(\xi(x))}{3!}$ above with

$$r(x) \coloneqq \frac{f(x) - p(x)}{w'(x)} \Rightarrow f(x) = p(x) + r(x)w'(x)$$

Similarly as the steps above, we can derive

$$\begin{aligned} Err &= \int_a^b f(x) - p(x)\,dx = \int_a^b r(x)w'(x)\,dx = [r(x)w(x)]_a^b - \int_a^b r'(x)w(x)\,dx && (2) \\ &= -r'(\xi) \int_a^b w(x)\,dx && (3) \end{aligned}$$

for some $\xi \in (a, b)$, where we applied the weighted Mean Value Theorem in the last step.

We can use Rolle's theorem to show that for each ξ there exists a $\eta \in (a, b)$ such that $r'(\xi) = \frac{f^{(4)}(\eta)}{4!}$. Then we can obtain the same answer. I will leave the details to you. ☺

Problem 2

Let $x_0 = -\sqrt{\frac{3}{5}}, x_1 = 0$, and $x_2 = \sqrt{\frac{3}{5}}$. Find weights w_0, w_1, and w_2 such that

$$\int_{-1}^{1} f(x)\,dx = w_0 f(x_0) + w_1 f(x_1) + w_2 f(x_2) \tag{4}$$

holds whenever f is a polynomial of degree less than or equal to 2. Show that the formula in fact holds when f is a polynomial of degree less than or equal to 5.

Ans: The three points x_0, x_1, x_2 given above are actually Gauss-Legendre quadrature rule with three points! Please refer back to lecture 19 and more on `https://en.wikipedia.org/wiki/Gaussian_quadrature`.

Same as the previous problem, we substitute $f_1(x) = 1, \quad f_2(x) = x, \quad f_3(x) = x^2$ into (4). We have

$$\begin{cases} 2 = \int_{-1}^{1} 1\,dx & = w_0 \cdot 1 + w_1 \cdot 1 + w_2 \cdot 1 \\ 0 = \int_{-1}^{1} x\,dx & = w_0 \cdot \left(-\sqrt{\frac{3}{5}}\right) + w_1 \cdot 0 + w_2 \cdot \left(\sqrt{\frac{3}{5}}\right) \\ \frac{2}{3} = \int_{-1}^{1} x^2\,dx & = w_0 \cdot \left(-\sqrt{\frac{3}{5}}\right)^2 + w_1 \cdot 0 + w_2 \cdot \left(\sqrt{\frac{3}{5}}\right)^2 \end{cases} \Rightarrow \quad w_0 = \frac{5}{9},\ w_1 = \frac{8}{9},\ w_2 = \frac{5}{9}$$

Alternatively, as shown in class, the Gauss-Legendre quadrature weights can be obtained via the Lagranage interpolation formula. Here I demonstrate how to calculate w_0 and you should be able to compute w_1, w_2 on your own:

$$\begin{aligned} w_0 &= \int_{-1}^{1} L_0(x)\,dx = \int_{-1}^{1} \prod_{\substack{0 \le i \le 2 \\ i \ne 0}} \frac{x - x_i}{x - x_0}\,dx = \int_{-1}^{1} \frac{x(x - \sqrt{\frac{3}{5}})}{\left(-\sqrt{\frac{3}{5}}\right)\left(-2\sqrt{\frac{3}{5}}\right)}\,dx \\ &= \frac{5}{6} \int_{-1}^{1} x\left(x - \sqrt{\frac{3}{5}}\right)dx = \frac{5}{6} \cdot \frac{2}{3} = \frac{5}{9} \end{aligned}$$

Now we want show that the quadrature rule (4) above is exact for any polynomials of degree up to (including equal to) 5.

As said, the given points x_0, x_1, x_2 given are Gauss-Legendre points of degree with $N = 2$. They are the roots of the Legendre polynomial of degree 3, $P_3(x) = \frac{5}{2}x^3 - \frac{3}{2}x$. Therefore, it is exact for polynomial of degree less than or equal to $2(2) + 1 = 5$ in our case.

Remark 2. For those of you who have difficulty in understanding the proof in class, I repeat the same proof for $N = 2$.

Assume we only know that the Gauss-Legendre quadrature (4) holds exactly for degree less than or equal to 2.

Suppose that p is a polynomial of degree 5. Then by the polynomial division, we can write $p(x) = q(x)P_3(x) + r(x)$, where $P_3(x) = \frac{3}{2}x^2 - \frac{1}{2}$ is the Legendre polynomial of degree 3, $q(x)$ a polynomial of degree at most 2 and $r(x)$ is a polynomial of degree at most 2.

Since the Legendre polynomials form an orthogonal basis for functions on interval $[-1,1]$ with respect to the L^2 inner product by construction, i.e.

$$\langle P_m, P_n \rangle = \int_{-1}^{1} P_m(x)P_n(x)\,dx = \begin{cases} \frac{2}{2n+1}, & m = n \\ 0, & m \neq n \end{cases}$$

The Legendre polynomial P_3 is orthogonal to any polynomials of degree up to (including equal to) 2, i.e. $\int_{-1}^{1} q(x)P_3(x)\,dx = 0$. So

$$\int_{-1}^{1} p(x)\,dx = \int_{-1}^{1} q(x)P_3(x) + r(x)\,dx = \int_{-1}^{1} r(x)\,dx$$

Since Gauss-Legendre quadrature holds exactly for degree less than or equal to 2 and x_0, x_1, x_2 are roots of $P_3(x)$, we have

$$\sum_{k=1}^{n} p(x_k)w_k = \sum_{k=1}^{n} \left(q(x_k)\underbrace{P_3(x_k)}_{=0} + r_(x_k) \right) w_k = \sum_{k=1}^{n} \underbrace{r(x_k)}_{deg(r)\leq 2}\, w_k = \int_{-1}^{1} r(x)\,dx = \int_{-1}^{1} p(x)\,dx$$

So (4) holds exactly for degree less than or equal to 5. The above proof cannot work for polynomials of degree higher than or equal to 6, why?

Problem 3

Let $x_0 = 0, x_1 = \frac{1}{2}, x_2 = 1$. Find weights w_0, w_1, and w_2 such that the formula

$$\int_{0}^{1} f(x)\sqrt{x}\,dx = w_0 f(x_0) + w_1 f(x_1) + w_2 f(x_2) \tag{5}$$

when f is a polynomial of degree less than or equal to 2. Use this quadrature rule to approximate

$$\int_{0}^{1} cos(x)\sqrt{x}\,dx$$

How accurate is your approximation?

Ans: We substitute $f_1(x) = 1,\ f_2(x) = x,\ f_3(x) = x^2$ into (5).

$$\begin{cases} 1 = \int_0^1 1\,dx & = w_0 \cdot 1 + w_1 \cdot 1 + w_2 \cdot 1 \\ \frac{2}{5} = \int_0^1 x\sqrt{x}\,dx & = w_0 \cdot 0 + w_1 \cdot \frac{1}{2} + w_2 \cdot 1 \\ \frac{2}{7} = \int_0^1 x^2\,dx & = w_0 \cdot 0 + w_1 \cdot \left(\frac{1}{2}\right)^2 + w_2 \cdot 1^2 \end{cases} \Rightarrow \quad w_0 = \frac{13}{35},\ w_1 = \frac{16}{35},\ w_2 = \frac{6}{35}$$

Set $f(x) = cos(x)$,

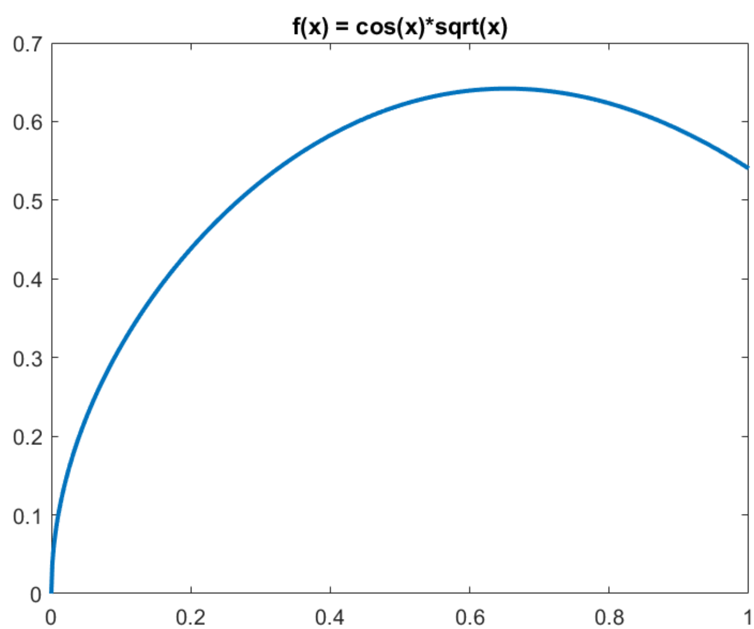
$$\int_0^1 f(x)\sqrt{x}\,dx = \frac{13}{35} f(0) + \frac{16}{35} f(\frac{1}{2}) + \frac{6}{35} f(1)$$
$$\Rightarrow \quad \int_0^1 cos(x)\sqrt{x}\,dx = \frac{13}{35} \cdot 1 + \frac{16}{35} \cdot cos\left(\frac{1}{2}\right) + \frac{6}{35} \cdot cos(1)$$

On one hand, using `MATLAB`, we compute the above sum to 15 decimal places $\approx 0.865232423584423$. On the other hand, using `Mathematica` , the exact value for this definite integral should be $\approx 0.531202683084515$.

The approximation is actually bad since it is wrong already in the first decimal place. The reason is the abrupt increase of the function $g(x) = cos(x)\sqrt{x}$ near $x = 0$ (*cos(x) is NOT a polynomial of any degrees!*), compute the derivative

$$g'(x) = -sin(x)\sqrt{x} + \frac{cos(x)}{2\sqrt{x}} \quad \Rightarrow \quad \lim_{x \to 0^+} g'(x) = +\infty$$

Below is a plot of $g(x)$ over $[0, 1]$, observe that the tangent line of $g(x)$ near $x = 0$ behaves like a vertical line.



Also, the error for Simpson rule should be bound by the term $\frac{h^5}{90}g^{(4)}(\xi)$. One can also show that the fourth derivative of $g(x)$ is unbounded as $x \to 0^+$. This also explains why the approximation is bad in this case.

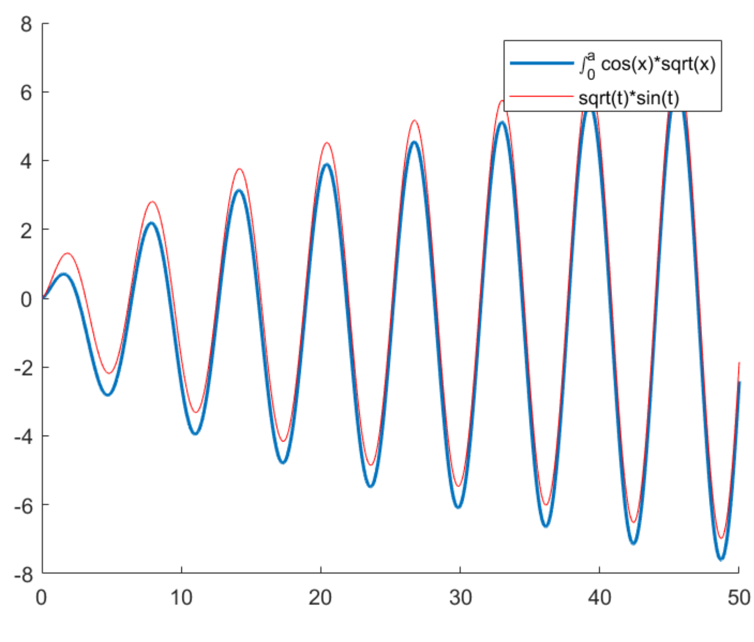
Bonus: For those who are interested in special integral, here is more to learn from this problem: If we look at our definite integral $F(a) \coloneqq \int_0^a cos(x)\sqrt{x}\,dx$ for real number $a \geq 0$, it seems hard to find a closed form (algebraic expressions) for this integral at first glance. But integrate by part and then use change of variable $x = t^2$, we have:

$$F(a) = \int_0^a cos(x)\sqrt{x}\,dx = \left[\sqrt{x}sin(x)\right]_0^a - \frac{1}{2}\int_0^a \frac{sin(x)}{\sqrt{x}}\,dx = \sqrt{a}sin(a) - \frac{1}{2}\int_0^{\sqrt{a}} \frac{sin(t^2)}{t}\,(2tdt)$$

$$\Rightarrow\ F(a) = \sqrt{a}sin(a) - \underbrace{\int_0^{\sqrt{a}} sin(t^2)\,dt}_{\coloneqq S(\sqrt{a})}$$

where $S(x) \coloneqq \int_0^x sin(t^2)\,dt$ is called the **Fresnel Integral** which has many interesting properties and is closely related to special curves. Please refer to https://en.wikipedia.org/wiki/Fresnel_integral for more info.

Lastly, our definite integral $F(x)$ has oscillatory behavior due to the dominant term $\sqrt{x}sin(x)$. Below is a plot showing a blue curve as $F(x)$ over the interval $[0, 50]$ and a red curve $g(x) = \sqrt{x}sin(x)$. The discrepancy between the two is due to the correction term, the Fresnel integral, $S(\sqrt{x})$.



Problem 4

Suppose that

$$f(x) = 2T_0(x) + 4T_1(x) - 6T_2(x) + 12T_3(x) - 14T_4(x)$$

Find

$$\int_{-1}^{1} f(x)\,dx$$

Ans: This should very straight-forward if you remember the integral formula for the n-th Chebyshev polynomial:

$$\int_{-1}^{1} T_n(x)\,dx = \begin{cases} 0, & n \text{ odd} \\ \frac{2}{1-n^2}, & n \text{ even} \end{cases}$$

The above formula holds for all $n = 0, 1, 2, \cdots$. This was the problem 4 in the midterm exam. Can you recall how to derive this formula? Make sure you can! ☺

So we have

$$\begin{aligned} \int_{-1}^{1} f(x)\,dx &= 2\int_{-1}^{1} T_0(x)\,dx + 4\cdot 0 - 6\int_{-1}^{1} T_2(x)\,dx + 12\cdot 0 - 14\int_{-1}^{1} T_4(x)\,dx \\ &= 2\frac{2}{1-0^2} - 6\frac{2}{1-2^2} - 14\frac{2}{1-4^2} = 4 + 4 + \frac{28}{15} = \frac{148}{15} \end{aligned}$$