Homework No.4, 553.481/681, Due March 19, 2021.

Problem 1. [DOUBLE] (a) Derive Boole's rule, the Newton-Cotes quadrature rule for $n = 4$, so that, with $x_i = a + ih$, $i = 0, .., 4$ for $h = (b - a)/4$, and $\xi \in [a, b]$

$$\int_a^b f(x)dx = \frac{2h}{45}\left[7f(x_0) + 32f(x_1) + 12f(x_2) + 32f(x_3) + 7f(x_4)\right] - \frac{8h^7}{945}f^{(6)}(\xi)$$

You do not need to evaluate by hand the integrals to determine the rational coefficients α_i, $i = 0, 1, ..., 4$ but instead you can use symbolic integration (for example, `int` in Matlab). To evaluate the error term, you should derive and use the expression

$$E_4(f) = \int_a^b f[x_0, x_1, x_2, x_3, x_4, x]\prod_{i=0}^{4}(x - x_i)$$

Then you can use without proof the fact that $w(x) := \int_a^x \prod_{i=0}^4(\bar{x} - x_i)\, d\bar{x} \geq 0$. The integral to determine the error coefficient can be again obtained symbolically.

Solution: We evaluate the following integrals:

$$\int_0^4 \frac{t-1}{0-1}\frac{t-2}{0-2}\frac{t-3}{0-3}\frac{t-4}{0-4}dt = \frac{14}{45}$$
$$\int_0^4 \frac{t-0}{1-0}\frac{t-2}{1-2}\frac{t-3}{1-3}\frac{t-4}{1-4}dt = \frac{64}{45}$$
$$\int_0^4 \frac{t-0}{2-0}\frac{t-1}{2-1}\frac{t-3}{2-3}\frac{t-4}{2-4}dt = \frac{24}{45}$$
$$\int_0^4 \frac{t-0}{3-0}\frac{t-1}{3-1}\frac{t-2}{3-2}\frac{t-4}{3-4}dt = \frac{64}{45}$$
$$\int_0^4 \frac{t-0}{4-0}\frac{t-1}{4-1}\frac{t-2}{4-2}\frac{t-3}{4-3}dt = \frac{14}{45}$$

To derive the forward difference, we can use a 6-th order approximation of the function:

$$f(x) = p_4(x) + f[x_0, x_1, x_2, x_3, x_4, x]\prod_{i=0}^{4}(x - x_i)$$
$$\int_a^b f(x)dx = \int_a^b p_4(x)dx + \int_a^b f[x_0, x_1, x_2, x_3, x_4, \epsilon]\prod_{i=0}^{4}(x - x_i)dx$$

So:

$$E_4(x) = \int_a^b f[x_0, x_1, x_2, x_3, x_4, \epsilon]\prod_{i=0}^{4}(x - x_i)dx$$

(b) Modify the course script `simpc.m` to write a code `boolc.m` that implements the composite Boole's rule.

(c) Use your code to compare the composite Simpson's rule and composite Boole's rule applied to the following two integrals:

$$\textit{(i)} \quad \int_0^1 dx \, \exp(-x^2) \qquad\qquad \textit{(ii)} \quad \int_{-4}^4 dx \, \frac{1}{1+x^2}.$$

Use $n = 8, 16, 32, 64, 128, 256$ and make a log-log plot of the errors in the approximations versus n. Are the results consistent with the proven asymptotic order of convergence? Explain your answer. For *(ii)* it may help to consider even larger n.

Note: The exact value of integral *(i)* can be obtained from the Matlab function `erf` and integral *(ii)* is $\int_{-4}^4 dx \, \frac{1}{1+x^2} = 2\arctan(4)$.

Solution: Images are in the folder. They are labeled "$prob_1c\_ < method > \_ < function >$". Function (i) is f and function (ii) is g. The convergence order I obtained for simpson's rule is n=4. The convergence order I obtained for Boole's rule is n=3. These do not match up with the theoretical results.

Problem 2. (a) Prove that the Bernoulli polynomials satisfy the following reflection property:

$$(-1)^j B_j(1-x) = B_j(x), \;\; j \geq 2.$$

Solution: We define the Bernoulli polynomials $B_k(x)$ with the generating function:

$$\frac{te^{xt}}{e^t - 1} = \sum_{k=0}^{\infty} B_k(x) \frac{t^k}{k!}$$

Now if we substitute $1 - x$ into the generating function, we get:

$$\frac{te^{(1-x)t}}{e^t - 1} = \frac{te^t e^{-tx}}{e^t - 1} = \frac{-te^{-tx}}{e^{-t} - 1} = \sum_{k=0}^{\infty} B_k(x) \frac{(-t)^k}{k!}$$

So we see that:

$$\sum_{k=0}^{\infty} B_k(1-x) \frac{t^k}{k!} = \sum_{k=0}^{\infty} (-1)^k B_k(x) \frac{(t)^k}{k!}$$

If we differentiate w.r.t. t a total of j times and set $t = 0$, we can solve for the j-th term:

$$(-1)^j B_j(1-x) = B_j(x)$$

(b) Prove the following identity relating the Bernoulli polynomials and Bernoulli numbers:

$$B_j'(x) = j[B_{j-1}(x) + B_{j-1}], \;\; j \geq 2.$$

We can again use the generating function. This time we take the derivative w.r.t x:

$$\frac{d}{dx} \frac{te^{xt}}{e^t - 1} = \sum_{k=0}^{\infty} B_k'(x) \frac{t^k}{k!}$$

When we evaluate the left side we get

$$\frac{d}{dx} \frac{te^{xt}}{e^t - 1} = \frac{t^2 e^{xt}}{e^t - 1} = t \left[\sum_{k=0}^{\infty} B_k(x) \frac{t^k}{k!} \right] = \sum_{k=0}^{\infty} B_k(x) \frac{t^{k+1}}{k!}$$

If we reparametrize the sum, we get:

$$\sum_{k=1}^{\infty} B_{k-1}(x)\frac{t^k}{(k-1)!}$$

Now we have the equality:

$$\sum_{k=0}^{\infty} B_k'(x)\frac{t^k}{k!} = \sum_{k=1}^{\infty} B_{k-1}(x)\frac{t^k}{(k-1)!}$$

Now we differentiate w.r.t. t a toal of j times and set $t = 0$ to find the j-th bernoulli polynomial:

$$B_j'(x) = jB_{j-1}(x)$$

Note: These results can be used to give a general proof of the Euler-MacLaurin formula. See Ralston, *A First Course in Numerical Analysis* (McGraw-Hill, 1965).

Problem 3. (a) The midpoint rule $I_M(f) = hf\left(\frac{a+b}{2}\right)$, $h = b - a$ for evaluating the integral $I(f) = \int_a^b f(x)\,dx$ can be shown to have the asymptotic error formula

$$I(f) = I_M(f) + \frac{h^2}{24}[f'(b) - f'(a)] + O(h^4).$$

Using this information, obtain a new numerical integration formula $\tilde{I}(f)$ with a higher order of convergence by making a linear combination of $I_M(f)$ and the trapezoidal rule $I_T(f) = \frac{h}{2}[f(a) + f(b)]$. Write out the weights for this new formula $\tilde{I}(f)$,

The error formula for the trapezoidal rule is:

$$I(f) = I_T(f) - \frac{h^2}{12}[f'(b) - f'(a)] + O(h^4).$$

So, a linear combination that reduces error is:

$$I(f) = \frac{2}{3}I_T(f) + \frac{1}{3}I_M(f)$$

(b) Show that in Romberg integration, with $T^{(0)}(h_k)$ the composite trapezoidal rule,

$$T^{(1)}(h_k) = \frac{1}{3}[4T^{(0)}(h_k) - T^{(0)}(h_{k-1})$$

is the composite Simpson rule and

$$T^{(1)}(h_k) = \frac{1}{15}[16T^{(1)}(h_k) - T^{(1)}(h_{k-1})$$

is the composite Boole rule.

Solution: We first start with the trapezoid rule:

$$T_n^{(0)} = \frac{1}{2} * h[f_0 + 2f_1 + 2f_2 + \ldots + 2f_{n-1} + f_n]$$

We can now sample at every $2h$ intervals instead. The new series is:

$$T_{n/2}^{(0)} = \frac{1}{2} * h[2f_0 + 4f_2 + 4f_4 + \ldots + 4f_{n-2} + f_n]$$

When we combine the series using the first Romberg formula:

$$\frac{1}{3}[4T_n^{(0)}(h_k) - T_{n/2}^{(0)}(h_{k-1})$$

When we combine the series according to this formula, we get:

$$\frac{h}{6}[[4f_0 + 8f_1 + 8f_2 + \ldots + 8f_{n-1} + 4f_n] - [2f_0 + 4f_2 + 4f_4 + \ldots + 4f_{n-2} + f_n])$$
$$= \frac{h}{3}[f_0 + 4f_1 + 2f_2 + \ldots + 4f_{n-1} + f_n]$$

This is the composite simpson's rule. To derive the composite Boole's rule, we start with Simpson's rule:

$$T_n^{(1)} = \frac{1}{3} * h[f_0 + 4f_1 + 2f_2 + \ldots + 4f_{n-1} + f_n]$$

We then sample at $2h$ rather than h, and get:

$$T_{n/2}^{(0=1)} = \frac{1}{3} * 2h[f_0 + 4f_2 + 2f_4 + \ldots + 4f_{n-2} + f_n]$$

Combining these together using the Romberg formula, we get:

$$\frac{h}{45}[16[f_0 + 4f_1 + 2f_2 + \ldots + 4f_{n-1} + f_n] - 2[f_0 + 4f_2 + 2f_4 + \ldots + 4f_{n-2} + f_n])$$
$$= \frac{h}{45}[14f_0 + 64f_1 + 24f_2 + 64f_3 + 14f_4 + 14f_4 + 64f_5 + \ldots 14f_n]$$
$$= \frac{2h}{45}[7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4 + 7f_4 + 32f_5 + \ldots 7f_n]$$

This is the composite Boole's Rule.

Problem 4. Use the MATLAB script `romberg.m` and the intrinsic function `quad` in order to compare Romberg integration and adaptive extrapolated Simpson's rule applied to the following integrals:

(i) $\int_0^4 dx\, \sin(x^2)$ *(ii)* $\int_{-2}^2 dx\, \exp[-\exp(x^{20})]$.

Calculate each integral to a tolerance of $tol = 10^{-14}$ and record the number of function calls made by both algorithms. Explain your results, using the geometric and smoothness properties of the integrands.

Solution: Function (i) has 1025 function calls, while (ii) has 16385 calls. This is because function (i) varis more continuously in the interval [0,4], where as function (ii) has a sharp turn at around $x = 1$.