Computational Physics – Problem Set 2

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October 1, 2019

1 Numerical Integration with Trapezoidal, Simpson, and 5-point formulas

- Trapezoidal rule

$$\int_{x_0}^{x_1} dx f(x) = \frac{h}{2}\Big(f(x_0) + f(x_1)\Big) - \frac{1}{12}h^3 f''(\xi)$$

- Simpson's rule

$$\int_{x_0}^{x_2} dx f(x) = \frac{h}{3}\Big(f(x_0) + 4f(x_1) + f(x_2)\Big) - \frac{1}{90}h^5 f^{(4)}(\xi)$$

- Boole's rule(5-point formulas)

$$\int_{x_0}^{x_4} dx f(x) = \frac{2h}{45}\Big(7f(x_0)+32f(x_1)+12f(x_2)+32f(x_3)+7f(x_4)\Big)-\frac{8}{945}h^7 f^{(6)}(\xi)$$

The above formulas can be derived from the Lagrange interpolating formula including the error term,

$$f(x) \approx P_n(x) \equiv \sum_{i=0}^{n} f(x_i)L_i(x) + \frac{f^{n+1}(\xi)}{(n+1)!}\prod_{i=0}^{n}(x - x_i),$$

where

$$L_i(x) = \prod_{j\neq i} \frac{x - x_j}{x_i - x_j}.$$

Another more accurate method is based on Taylor expansion around the middle point (if the number of point is odd) with error term up to the next order. For example, for the Boole's rule, one takes the five points x_0, x_1, x_2, x_3, x_4 and makes the expansion around x_2:

$$
\begin{aligned}
f(x) = f(x_2) + f'(x_2)(x-x_2) + \frac{f''(x_2)}{2!}(x-x_2)^2 + \frac{f^{(3)}(x_2)}{3!}(x-x_2)^3 \\
+ \frac{f^{(4)}(x_2)}{4!}(x-x_2)^4 + \frac{f^{(5)}(x_2)}{5!}(x-x_2)^5 + \frac{f^{(6)}(\xi)}{6!}(x-x_2)^6.
\end{aligned}
$$

The integration from x_0 to x_4 gives:

$$
\begin{aligned}
\int_{x_0}^{x_4} dx f(x) = \int_{x_0}^{x_4} dx f(x_2) + f'(x_2)\int_{x_0}^{x_4} dx(x-x_2) + \frac{f''(x_2)}{2!}\int_{x_0}^{x_4} dx(x-x_2)^2 \\
+ \frac{f^{(3)}(x_2)}{3!}\int_{x_0}^{x_4} dx(x-x_2)^3 + \frac{f^{(4)}(x_2)}{4!}\int_{x_0}^{x_4} dx(x-x_2)^4 \\
+ \frac{f^{(5)}(x_2)}{5!}\int_{x_0}^{x_4} dx(x-x_2)^5 + \frac{f^{(6)}(\xi)}{6!}\int_{x_0}^{x_4} dx(x-x_2)^6.
\end{aligned}
$$

$$
\int_{x_0}^{x_4} dx f(x) = 4hf(x_2) + \frac{1}{3}(2h)^3 f''(x_2) + \frac{2}{5}(2h)^5\frac{f^{(4)}(x_2)}{4!} + \frac{2}{7}(2h)^7\frac{f^{(6)}(\xi)}{6!}.
$$

From the 3-point formula for the second derivative of a function,

$$
\begin{aligned}
f''(x_2) &= \frac{f(x_3) - 2f(x_2) + f(x_1)}{h^2} - \frac{h^2}{12}f^{(4)}(x_2) - \frac{h^4}{360}f^{(6)}(\xi) \\
f''(x_2) &= \frac{f(x_3) - 2f(x_2) + f(x_1)}{(2h)^2} - \frac{(2h)^2}{12}f^{(4)}(x_2) - \frac{(2h)^4}{360}f^{(6)}(\xi)
\end{aligned}
$$

one can obtain $f''(x_2)$ to the forth order,

$$
f''(x_2) = \frac{-f(x_4) + 16f(x_3) - 30f(x_2) + 16f(x_1) - f(x_0)}{12h^2} + \frac{h^4}{30}f^{(6)}(\xi),
$$

and

$$
f^{(4)}(x_2) = \frac{f(x_4) - 4f(x_3) + 6f(x_2) - 4f(x_1) + f(x_0)}{h^4} - \frac{h^2}{6}f^{(6)}(\xi).
$$

Plug them to the integral with 5 points, one obtains the Boole's rule.

In the first problem, we would like to evaluate

$$
\int_0^{\pi} dx sin(x).
$$

To do this, one uses the above approximation rule several times(assume N is the mutiple of 4).

- Extended trapezoidal rule

$$\int_{x_0}^{x_N} dx f(x) = \left(\int_{x_0}^{x_1} + \int_{x_1}^{x_2} + ... + \int_{x_{N-1}}^{x_N} \right) dx f(x)$$

$$= h\left(\frac{1}{2} f_0 + f_1 + ... + f_{N-1} \frac{1}{2} f_N \right) - \frac{1}{12} N h^3 f''(\xi)$$

- Extended Simpson's rule

$$\int_{x_0}^{x_N} dx f(x) = \left(\int_{x_0}^{x_2} + \int_{x_2}^{x_4} + ... + \int_{x_{N-2}}^{x_N} \right) dx f(x)$$

$$= \frac{1}{3} h\left(f_0 + 4f_1 + 2f_2 + ... + 4f_{N-1} + f_N \right) - \frac{1}{90} \frac{N}{2} h^5 f''(\xi)$$

- Extended Boole's rule

$$\int_{x_0}^{x_N} dx f(x) = \left(\int_{x_0}^{x_4} + \int_{x_4}^{x_8} + ... + \int_{x_{N-4}}^{x_N} \right) dx f(x)$$

$$= \frac{2}{45} h\left(7f_0 + 32f_1 + 12f_2 + 32f_3 + 14f_4 + ... + 32f_{N-1} + 7f_N \right) - \frac{8}{945} \frac{N}{4} h^7 f''(\xi)$$

Below is the table of the deviation of different rules from the exact value of the integral, which is 2. In general, as expected, the 5-point formula gives the better approximation of the integral, since the error term of Boole's rule is up to h^7.

N	Trapezoidal	Simpson	Boole
4	0.1038811207	0.0045599937	0.0014292002
8	0.0257682800	0.0002691746	0.0000169277
16	0.0064297915	0.0000166893	0.0000004768
32	0.0016074181	0.0000004768	0.0000004768
64	0.0004006624	0.0000007153	0.0000007153
128	0.0001002550	0.0000001192	0.0000001192
256	0.0000286102	0.0000035763	0.0000036955
512	0.0000121593	0.0000042915	0.0000051260
1024	0.0000063181	0.0000051260	0.0000042915

2 Romberg Integration

For Romberg integration, start with the trapezoidal rule:

$$T_{m,0} = h\left(\frac{f_0}{2} + f_1 + ... + f_{N-1} + \frac{f_N}{2}\right).$$

Then according to the iteration formula:

$$T_{m+k,k} = \frac{4^k T_{m+k,k-1} - T_{m+k-1,k-1}}{4^k - 1},$$

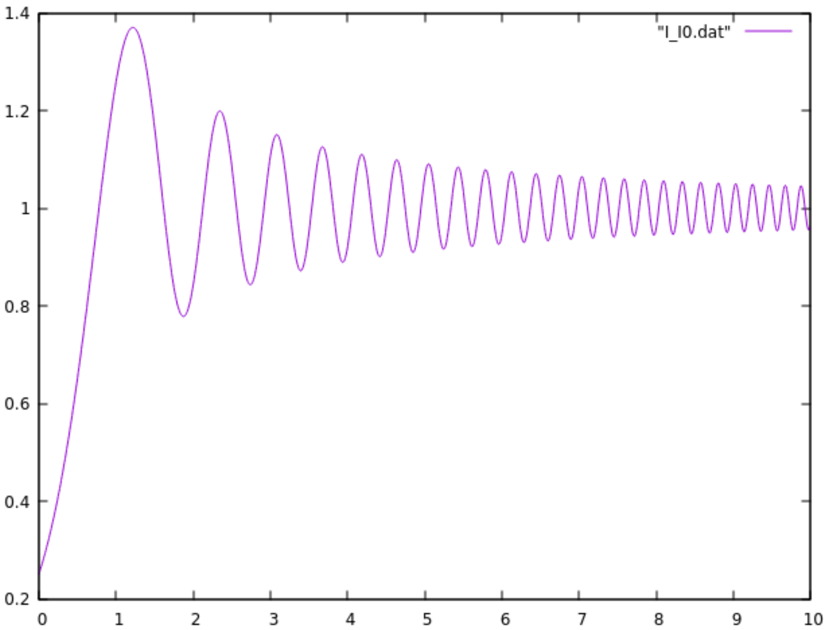
one can write the code below to perform the iteration for the integral. On the line 17 to 21, I want to check whether the Romberg integration works according to:

$$R_m = \frac{T_{m-1,0} - T_{m,0}}{T_{m,0} - T_{m+1,0}} \approx 4$$

```
1  /*  Romberg integration :
2   *  integrate function f from a to b with max iteration steps max_steps */
3  float Romberg(float **R, float (*f)(float),float a,float b, size_t max_steps,float acc, float *R_check){
4      int N = 1<<5;
5      for (size_t i = 0; i < max_steps; ++i){
6          R[i][0] = Trapezoid((*f), N, a, b);
7  
8          for (size_t j = 1; j <= i; ++j){
9              R[i][j] = (pow(4,j)*R[i][j-1] - R[i-1][j-1])/(pow(4,j) - 1);
10         }
11 
12         if (i > 0 && fabs(R[i][i] - R[i-1][i-1]) < acc)
13             return R[i][i];
14         N *= 2;
15     }
16 
17     for(size_t i = 1; i < max_steps - 1; ++i){
18         R_check[i] = (R[i-1][0] - R[i][0])/(R[i][0] - R[i+1][0]);
19     }
20     R_check[0] = 0;
21     R_check[max_itstep - 1] = 0;
22 
23 
24     return R[max_steps-1][max_steps-1];
25 }
```

In the second problem, the integral we would like to evaluate is

$$C(\nu) = \int_0^\nu dw cos\left(\frac{\pi w^2}{2}\right), S(\nu) = \int_0^\nu dw sin\left(\frac{\pi w^2}{2}\right)$$



Here, I plot

$$\frac{I}{I_0} = \frac{1}{2}\left((C(\nu) + 0.5)^2 + (S(\nu) + 0.5)^2\right)$$

as the function of ν, ranging from 0 to 10.

The Romberg check at $\nu = 4.77 - 4.82$ is:

m / ν	4.77	4.78	4.79	4.80	4.81	4.82
2	4.338214	4.466623	4.602847	4.077215	4.272999	4.316915
3	4.083204	4.240892	4.114053	3.593963	3.908495	4.157397
4	3.995094	4.185833	18.185184	2.060869	3.073088	4.039226

As expected, the R_m is roughly equal to 4, except for some irregular points.