Homework 9

Yifan Zhong

May 17, 2018

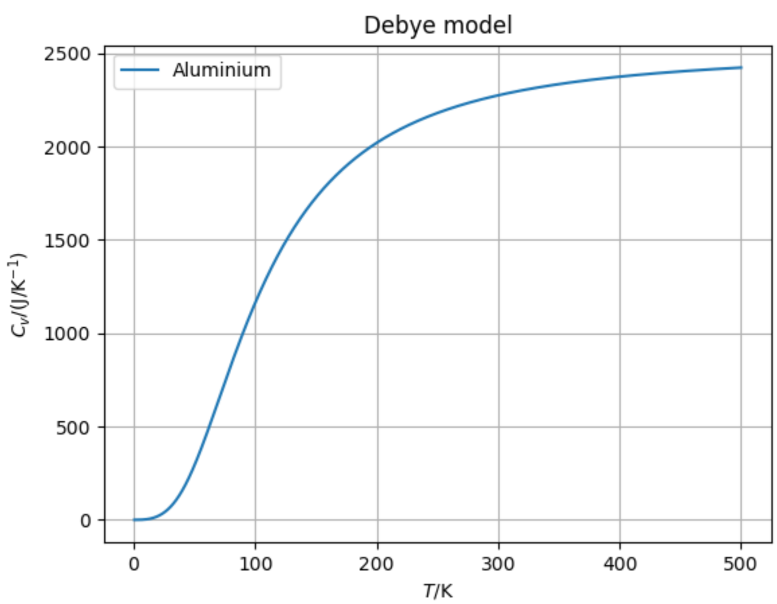
1 Problem 1

In this problem, Simpson's method is performed to evaluate the integral

$$C_V = 9V\rho k_b \left(\frac{T}{\theta_D}\right) \int_0^{\frac{\theta_d}{T}} \frac{x^4 e^x}{(e^x - 1)^2} dx$$

Thus we can attain Debye's solid heat capacity. The heat capacity is plotted in the from 5K to 500K as following

Figure 1: Debye Model



2 Problem 2

In this section, I compared the precision of trapezoidal method and Simpson's method using the same integral

$$I = \int_0^1 \sin^2(10\sqrt{x})dx$$

To achieve $\varepsilon = 10^{-10}$ Simpson's method requires 1964 sub-intervals while trapezoidal method needs 282012 sub-intervals. We can conclude that Simpson's method performs far better.

3 Problem 3

In this section, I will check the theoretical error bound of trapezoidal rule, Simpson's rule and Romberg's rule. It is quite straightforward. Fitting the error and the number of panels in log scale will give us the result.

However, for the given integrand the lecture note, the error bound is different from the general one.

3.1 Trapezoidal Rule

The error bound for trapezoidal rule is

$$E_T = \frac{|b-a|}{12n^2} f''(\xi)$$

and the experimental plot is

The slope in of the line is -2.01 in Figure 2. This is in accordance with the error is inversely proportional to the square of the number of panels. Our theory is verified.

3.2 Simpson's Rule

The error bound for Simpson's rule is

$$E_S = \frac{|b-a|}{180n^4} f^{(4)}(\xi) \tag{1}$$

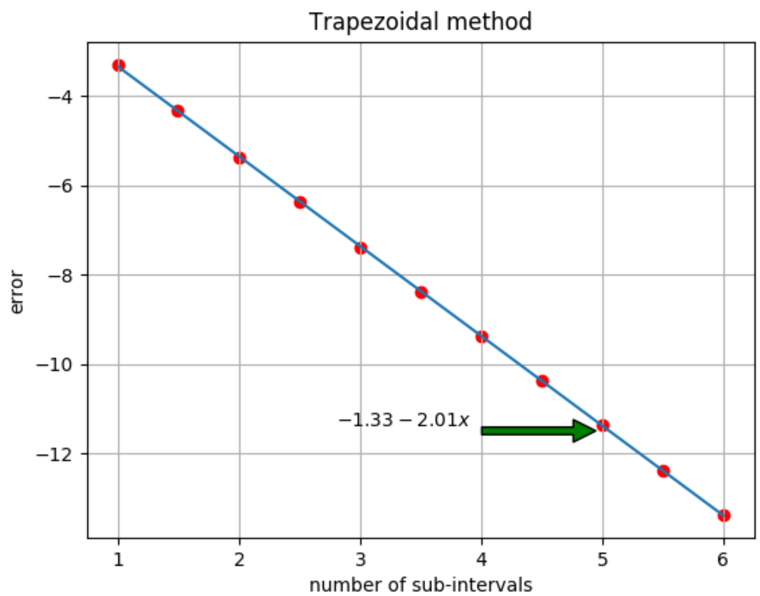
However my result is This slope is approximately -6 in the plot. A further examination on the integrand will explain the phenomenon. The function is:

$$f(x) = \frac{1}{1+x^2} \tag{2}$$

For an asymptotic error estimate, Equation 1 may be written into

$$E_S = \frac{|b-a|}{180n^4} [f^{(3)}(b) - f^{(3)}(a)] \tag{3}$$

Figure 2: Trapezoidal Rule



The derivatives at the endpoint of the interval gives

$$f^{(3)}(b) = f^{(3)}(a) = 0$$

Therefore, the error bound given by Equation 1 should be corrected. Since the we average the approximation over $[a, b]$ the error is a even function, The next term is proportional to $1/n^6$. This is the reason for the slope to be -6

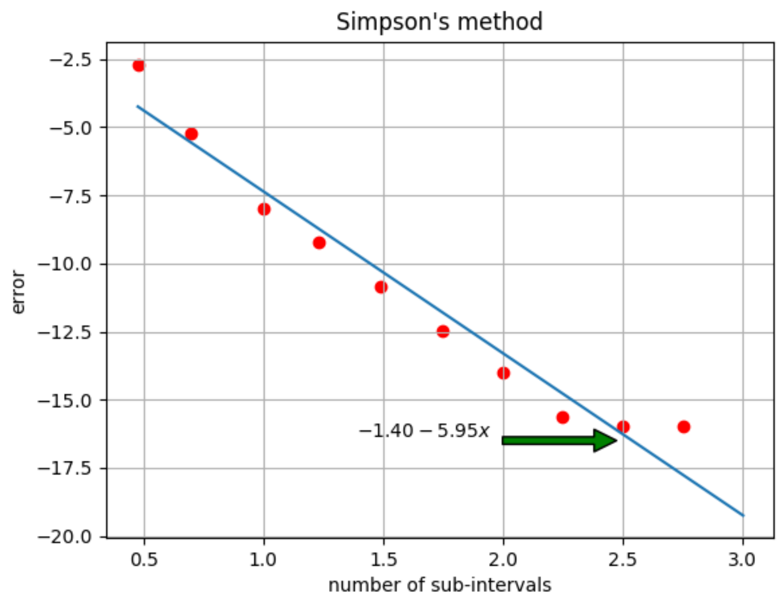
Here is a more detailed derivation. Consider the integration over the panel $x_j \leq x < x_j + 2h$. Simpson's rule gives

$$\int_{x_j}^{x_j+2h} f(x)dx \approx \frac{h}{3}\left(f_j + 4f + f_{j+2}\right) \tag{4}$$

We may rearrange the rule by expressing f_j and f_{j+2} via f. This can be easily achieved by Taylor expansion.

$$\begin{aligned} f_j &= f(x_{j+1} - h) \qquad (5) \\ &= f\left(x_{j+1}\right) - hf'\left(x_{j+1}\right) + \frac{1}{2}h^2 f''\left(x_{j+1}\right) - \frac{1}{6}h^3 f^{(3)}\left(x_{j+1}\right) + \frac{1}{24}h^4 f^{(4)}\left(x_{j+1}\right) \\ &- \frac{1}{120}h^5 f^{(5)}\left(x_{j+1}\right) + \frac{1}{720}h^6 f^{(6)}\left(x_{j+1}\right) + O\left(h^7\right) \end{aligned}$$

Figure 3: Simpson's Rule



$$\begin{aligned}
f_j &= f(x_{j+1} - h) \qquad (6)\\
&= f\left(x_{j+1}\right) + hf'\left(x_{j+1}\right) + \frac{1}{2}h^2 f''\left(x_{j+1}\right) + \frac{1}{6}h^3 f^{(3)}\left(x_{j+1}\right) + \frac{1}{24}h^4 f^{(4)}\left(x_{j+1}\right)\\
&+ \frac{1}{120}h^5 f^{(5)}\left(x_{j+1}\right) + \frac{1}{720}h^6 f^{(6)}\left(x_{j+1}\right) + O\left(h^7\right)
\end{aligned}$$

Substitute Equation 6 and 7 into 4, we have:

$$\int_{x_j}^{x_j+2h} f(x)dx \approx 2h\left(f + \frac{1}{3}\frac{h^2}{2!}f''\left(x_{j+1}\right) + \frac{1}{3}\frac{h^4}{4!}f''\left(x_{j+1}\right) + \frac{1}{3}\frac{h^6}{6!}f^{(6)}\left(x_{j+1}\right)\right) \qquad (7)$$

On the other hand, we can expand $f(x)$ directly at x_{j+1}

$$\begin{aligned}
f(x) &\approx f\left(x_{j+1}\right) + hf'\left(x_{j+1}\right) + \frac{1}{2!}h^2 f''\left(x_{j+1}\right) + \frac{1}{3!}h^3 f^{(3)}\left(x_{j+1}\right) \qquad (8)\\
&+ \frac{1}{4!}h^4 f^{(4)}\left(x_{j+1}\right)\frac{1}{5!}h^5 f^{(5)}\left(x_{j+1}\right) + \frac{1}{6!}h^6 f^{(6)}\left(x_{j+1}\right) + O\left(h^7\right)
\end{aligned}$$

The integral would be

$$\int_{x_j}^{x_j+2h} f(x)dx \approx 2h\left(f + \frac{1}{3}\frac{h^2}{2!}f''\left(x_{j+1}\right) + \frac{1}{5}\frac{h^4}{4!}f^{(4)}\left(x_{j+1}\right) + \frac{1}{7}\frac{h^6}{6!}f^{(6)}\left(x_{j+1}\right)\right) \qquad (9)$$

Comparing Equation 7 and 9 immediately yields the error bound with two terms

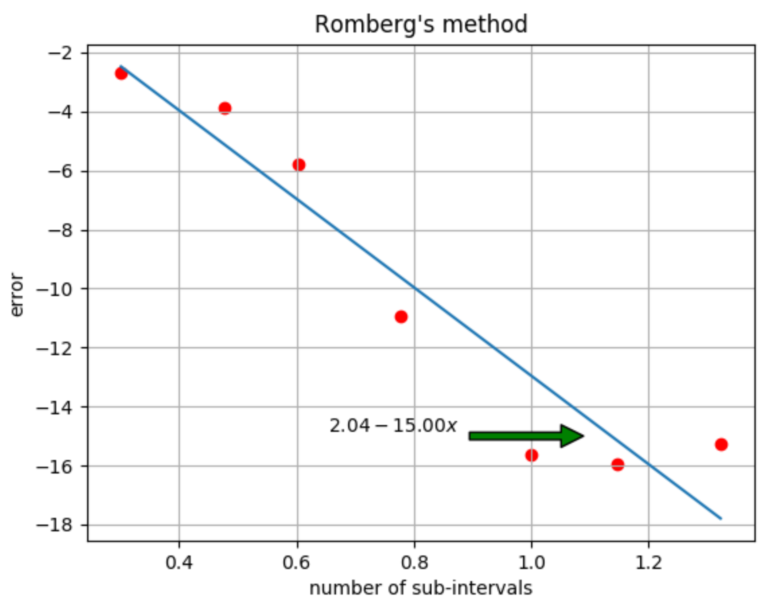
$$R_S = 2h\left[\left(\frac{1}{5}-\frac{1}{3}\right)\frac{h^4}{4!}f^{(4)}\left(x_{j+1}\right)+\left(\frac{1}{7}-\frac{1}{3}\right)\frac{h^4}{4!}f^{(6)}\left(x_{j+1}\right)\right] \tag{10}$$

For the same reason in Equation 3, the first term in Equation 10 is cancelled due to the special behaviour of the integrand in our case. Thus the overall error is inversely proportional to n^6

3.3 Romberg Integration

The error of Romberg integration is plotted as follows

Figure 4: Romberg Integration



4 Running the Scripts

All the scripts can be simply invoked by running the script “main.py”. You can run them individually as well.