PHYS 3142 HW 9

Due date: 11:59 PM 17$^{\text{th}}$ Apr. 2022

- Submit a report that includes your results and your python scripts
- Make sure your code can run
- Write comments in your code
- If you submit the assignment after the deadline or the report is missing, you can only get at most 80% of the full marks.
- If there is any kind of plagiarism, all students involved will get zero marks.

1 Ferromagnetism (50 points)

In the mean-field theory of ferromagnetism, the strength of magnetization M of a ferromagnetic material like iron depends on temperature T according to the formula

$$M = \mu \tanh \frac{JM}{k_B T}, \tag{1}$$

where μ is a magnetic moment, J is a coupling constant, and k_B is Boltzmann's constant. To simplify the expression, define $x = M/\mu$ and $C = \frac{\mu\ J}{k_B}$ so that

$$x = \tanh \frac{Cx}{T} \tag{2}$$

The magnetization x (which is in units of μ) can be solved using the relaxation method. Denote x after i iterations as x_i, the initial guess as x_0.

1. a Let $C = 1$. Use $x_0 = 1$ as your initial guess. Using 50 iterations in the relaxation method at each temperature, plot the temperature dependence of x from $T = 0.1$ to $T = 2$. The plot shows that equation 2 describes a phase transition.

1. b Following p. 10 of lecture 16, denote the accurate solution as x^*, the error for x_i is $\epsilon_i = |x_i - x^*|$.

Start from $x_i - x^* = f(x_{i-1}) - x^*$ and Taylor expand $f(x_{i-1})$ at x^*, derive the estimation of the error

$$\epsilon_i \approx \left| \frac{(x_{i-1} - x_i)^2}{2x_{i-1} - x_{i-2} - x_i} \right| \tag{3}$$

Assume that after a few iterations $|x_i - x_{i-1}|$ is small, and the derivative at x^* can be approximated using backward difference at x_{i-1}.

$$f'(x^*) \approx f'(x_{i-1}) \approx \frac{f(x_{i-1}) - f(x_{i-2})}{x_{i-1} - x_{i-2}} \tag{4}$$

1. c For $C = 1$, $T = 0.9$ and $x_0 = 1$, first estimate x^* using 50 iterations. Plot the actual error $|x_i - x^*|$ and the estimation from eq. 3 in the same figure. Start with $i = 5$ up to $i = 30$. This shows the validity of the estimation. Also, plot the graph using log scale for the error (use `plt.semilogy()`) to show that the error decreases exponentially.

1. d Plot the actual error $|x - x^*|$ for relaxation method and for over-relaxation method (with $\omega = 1$) in the same figure. Estimate x^* using 50 iterations in the over-relaxation method. Other parameters are the same as in 1. c.

2 Wien's displacement law (50 points)

Planck's radiation law tells us that the intensity of radiation per unit area and per unit wavelength λ from a black body at temperature T is

$$I(\lambda) = \frac{2\pi hc^2\lambda^{-5}}{e^{hc/(\lambda k_B T)} - 1} \tag{5}$$

Denote the λ that gives the maximum $I(\lambda)$ as λ_{peak}. Wien's displacement law states that

$$\lambda_{peak} = \frac{b}{T} \tag{6}$$

For example, this law can be used to estimate the temperature of the sun.

Define $x = \frac{hc}{\lambda k_B T}$ $(x > 0)$, omitting the proportionality constants, $I(x) \propto f(x)$, with

$$f(x) = \frac{x^5}{e^x - 1} \tag{7}$$

Denote the x with maximum $I(x)$ (for $x > 0$) as x_{peak}, the Wien's displacement constant is $b = \frac{hc}{k_B x_{peak}}$.

2. a Write down $\frac{df(x)}{dx}$ analytically. Plot $f(x)$ and $\frac{df(x)}{dx}$ on the same figure. Use a range of x from $x = 0.1$ to $x = 20$. Also plot a horizontal dashed line at $y = 0$. x_{peak} is the root of $\frac{df(x)}{dx}$ near $x = 5$.

2. b Write down $\frac{d^2f(x)}{dx^2}$ analytically. Use Netwon's method to find the root of $\frac{df(x)}{dx}$. Estimate the error from the i^{th} iteration as $\epsilon_i \approx |x_{i+1} - x_i|$. Try some values of x_0, if the correct x_{peak} cannot be reached, what x do you have instead? Why the update fails for $x = 0$? Using $x_0 = 5$, how many iterations do you need to have $\epsilon_i < 10^{-6}$? Write down that x_i.

2. c Use Golden's ratio search to find the maximum of $f(x)$. Denote i as how many times you redefine x_1 or x_4, and $\epsilon_i = x_4 - x_1$. Using $x_1 = 0.1$ and $x_4 = 20$ to start the search, how many iterations do you need to have $\epsilon_i < 10^{-6}$? Write down $(x_1 + x_4)/2$ after that accuracy is reached. Make sure the result agrees with parts **a** and **b**.

2. d Give at least one advantage and one disadvantage for each of the two methods. You can comment on the accuracy, the stability or other aspects.

Optional

3 Gradient descent method (10 points)

The numerical gradient descent method is

$$x_i = x_{i-1} - \gamma \frac{f(x_{i-1}) - f(x_{i-2})}{x_{i-1} - x_{i-2}} \tag{8}$$

You have 3 parameters, γ, x_0 and x_1. Use the $f(x)$ in question 2. Try different γ, x_0, x_1 and plot all the x_i (for $i \leq 30$) to determine if x_i converges or not. When you find suitable parameters, attach the plot in your report.

Plot $\frac{d^2 f(x)}{dx^2}$. Comment on how to choose a suitable γ. How to choose the sign and the magnitude of γ?