Indian Institute of Technology, Madras
Department of Applied Mechanics & Biomedical Engineering
Computational Tools: Algorithms, Data Structures and Programs - ID6105

Assignment set - VI

To be submitted by: Thursday 30^{th} October, 2025.

1 Problem 1

Find the gradient vector and Hessian matrix for each of the following functions:
(a)) $f(x, y) = 2xy^2 + 3e^{xy}$,
(b) $f(x, y, z) = x^2 + y^2 + 2z^2$,
(c) $f(x, y) = \ln(x^2 + 2xy + 3y^2)$,

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2 Problem 2

Compare two different methods of optimization, one given by steepest descent/ascent method and the other by Newton's method for the following set of problems. Stop when you have less than 1% change (stopping criteria),
(a) find the minimum value of $f(x, y) = (x - 3)^2 + (y - 2)^2$, starting at $x = 1$ and $y = 1$.
(b) find the maximum value of $f(x, y, z) = x^2 + y^2 + 2z^2$, starting at $x = 0$ and $y = 0$.
(c) find the minimum value of $f(x, y) = \ln(x^2 + 2xy + 3y^2)$, starting at $x = 0$ and $y = 0$.
Which method is faster for each problem and why?

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3 Problem 3

Evaluate the following integral analytically:

$$\int_0^3 x^2 e^{2x} dx \tag{1}$$

and also evaluate numerically with the following methods,
(a) single application of trapezoidal rule across $0 - 3$,
(b) multiple-application of trapezoidal rule, with $n = 2$ and 4, n here representing the number of equal intervals,

(c) single application of Simpson's 1/3 rule,
(d) multiple-application Simpson's 1/3 rule, with $n = 4$,
(e) single application of Simpson's 3/8 rule,
(f) multiple-application Simpson's 3/8 rule, with $n = 5$.
For each of the numerical estimates determine the percent relative error based on the analytical value.

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4 Problem 4

A transportation engineering study requires that you determine the number of cars that pass through an intersection traveling during morning rush hour. You stand at the side of the road and count the number of cars that pass every 4 minutes at several times as tabulated in table 1. Use the best numerical method to determine,
(a) the total number of cars that pass between 7:30 and 9:15, and
(b) the rate of cars going through the intersection per minute.

Time (hr)	7:30	7:45	8:00	8:15	8:45	9:15
Rate (cars per 4 mins)	18	24	26	20	18	9

Table 1: Traffic data

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5 Problem 5

There is no closed form solution for the error function,

$$\text{erf}(x) = \int_0^x e^{-x^2/2} dx \tag{2}$$

Use the Rhomberg integration and two-point Gauss quadrature approach to estimate erf(1.5). Note that the exact value is 0.966105.

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6 Problem 6

Using the Taylor-Series expansion, find the exact form of the error term ϵ in the approximation below,

$$f'(x) \approx \frac{f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)}{12h} + \mathcal{O}(\epsilon). \tag{3}$$

Write your solution as a series of terms with derivatives evaluated at x.

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7 Problem 7

The Rosin-Rammler-Bennet (RRB) equation is used to describe size distribution in fine dust. F(x) represents the cumulative mass of dust particles of diameter x and smaller. x' and n' are constants equal to $30\mu m$ and 1.44, respectively. The mass density distribution $f(x)$ or the mass of dust particles of a diameter x is found by taking the derivative of the cumulative distribution

$$F(x) = 1 - e^{-(x/x')^{n'}}, \qquad f(x) = \frac{dF(x)}{dx} \tag{4}$$

(a) Numerically calculate the mass density distribution $f(x)$ and plot both $f(x)$ and the cumulative distribution $F(x)$.

(b) Calculate the mode size of the mass density distribution $f(x)$, which is given by the size at which the derivative $f(x)$ is zero.

(c) Find the surface area per mass of the dust $S_m(cm^2/g)$ using

$$S_m = \frac{6}{\rho} \int_{d_{\min}}^{\infty} \frac{f(x)}{x} dx \tag{5}$$

The equation is valid only for spherical particles. Assume a density $\rho = 1g\,cm^{-3}$ and a minimum diameter of dust included in the distribution $d_{\min}$ of $1\mu m$.

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8 Problem 8

The logistic model is used to simulate population as in

$$\frac{dp}{dt} = k_{gm}(1 - p/p_{\max})p \tag{6}$$

where p= population, k_{gm} = the maximum growth rate under unlimited conditions, and $p_{\max}$ = the carrying capacity of the planet. Simulate the world's population from 1950 to 2025 using one of the numerical methods discussed in the course. Employ the following initial conditions and parameter values for your simulation: p_0 (in 1950)= $2,555$ million people, $k_{gm} = 0.026/yr$, and $p_{\max} = 12,000$ million people. Have the function generate output corresponding to the dates for the following measured population data. Develop a plot of your simulation along with the data shown in table 2. How does the population prediction for the year 2025 compare with the UN estimate for the current year?

Year	1950	1960	1970	1980	1990	2000
Population (in millions)	2555	3040	3708	4454	5276	6079

Table 2: Population data

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9 Problem 9

The following ODEs have been proposed as a model of an epidemic:

$$\begin{cases} \frac{dS}{dT} = -a\,S\,I, \\ \frac{dI}{dt} = a\,S\,I - r\,I, \\ \frac{dR}{dt} = r\,I, \end{cases} \tag{7}$$

where S = the susceptible individuals, I = the infected, R = the recovered, a = the infection rate, and r = the recovery rate. A city has $10,000$ people, all of whom are susceptible.

(a) If a single infectious individual enters the city at t = 0, compute the progression of the epidemic until the number of infected individuals falls below 10. Use the following parameters: $a = 0.002/(\text{person}\cdot\text{week})$ and $r = 0.15/\text{d}$. Develop time- series plots of all the state variables. Also generate a phase- plane plot of S versus I versus R.

(b) Suppose that after recovery, there is a loss of immunity that causes recovered individuals to become susceptible. This reinfection mechanism can be computed as ρR, where ρ = the reinfection rate. Modify the model to include this mechanism and repeat the computations in (a) using $\rho = 0.015/\text{d}$.
