P452 / P752 / PH652 Computational Physics

End-Semester examination, 2024

NISER, Bhubaneswar

Full marks: 40 | Time: 3 hours

Marks are given in **boldface** along with the questions. Attempt all.

- Show necessary calculations, if needed, in the exam copy.
- Comment on the accuracy (if relevant) of the outcome of your code.
- Append the code generated I/O at the end of your corresponding code under comments section.
- Question may not explicitly ask for plot(s), but still you have to supplement your answer with plot(s) where ever necessary.

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1. Consider a decaying radioactive source whose activity is measured at intervals of 15 seconds. The time (t in sec), total counts during each period (N) and uncertainties in counts ($\sigma(N) = \sqrt{N}$) is given in the file `endsemfit.txt` as columns. Use χ^2 linear regression to determine the lifetime (along with its error) of this source. Is the fit acceptable at 5% level of significance? (Take $\sigma(\ln N) = 1/\sqrt{N}$) **[6]**

2. Consider the `van der Waals` equation of state

$$\left(p + \frac{a}{V^2}\right)(V - b) = RT$$

Use `fixed point method` to compute volume V to an accuracy of 10^{-5} of Cl_2 at a temperature of $T = 300\,\mathrm{K}$, given $p = 5.95$ atm, $R = 0.0821$, $a = 6.254$ and $b = 0.05422$ (all in appropriate units). You may get two different solutions if you try doing it with two different fixed-point equations. Why? **[4+1]**

3. Prove the following statement for a 2×2 system : `The solution vector` $\mathbf{x}^\star$ `of the equation` $\mathbf{Ax} = \mathbf{b}$`, where` $\mathbf{A}$ `is positive definite and symmetric, is the minimal value of the quadratic form` **[4]**

$$f(\mathbf{x}) = \frac{1}{2}\langle \mathbf{x}, \mathbf{Ax}\rangle - \langle \mathbf{x}, \mathbf{b}\rangle$$

4. Householder reflector is a symmetric matrix of the form $\mathbf{P} = \mathbb{I} - \tau\,\mathbf{v}\mathbf{v}^T$. It reflects a nonzero vector $\mathbf{x}$ in a hyperplane which is perpendicular to the vector $\mathbf{v}$ *i.e.* $\mathbf{P}\,\mathbf{x}$ is the reflected vector.

   (a) Determine τ so that $\mathbf{P}$ becomes orthogonal. **[2]**

   (b) Using a 2×2 system, where $\mathbf{v} = [1\;\;0]^T$ and $\mathbf{x} = [1\;\;2]^T$, prove the above statement on reflection. **[2]**

5. Consider the 5×5 tridiagonal matrix given in the file `endsemmat.txt`. Using Power iteration method, verify that the first two largest eigenvalues and their corresponding eigenvectors of the matrix satisfy

$$\lambda_k = b + 2\sqrt{ac}\cos\left(\frac{k\pi}{n+1}\right) \quad \text{and} \quad v_k^i = 2\left(\sqrt{\frac{c}{a}}\right)^k \sin\left(\frac{ik\pi}{n+1}\right)$$

where $a = c = -1$, $b = 2$, $n = 5$, $k = 1, 2, \ldots 5$ and i is the i-th component of the k-th eigenvector. In case of any discrepancies, discuss its possible source(s). [**4+4**]

6. Use accept / reject method to generate pRNG distributed as

$$p(x) = 0.5\,\left(a^2 - x^2\right) \quad \text{for } |x| < a, \quad \text{where } a = 2 \tag{1}$$

and zero otherwise. You may use Gaussian distributed sample pdf $g(x)$ and system generated pRNG's. Comment on the success success probability. [**7**]

7. Use variational Monte Carlo to solve simple harmonic oscillator using the trial wavefunction in equation (1) with a being the variational parameter. Use at least 20 equally spaced a-values and 20k Monte Carlo steps. [**6**]