KFU Graz
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Computational Physics WS 24-25

You are allowed to use paper and pencil.

Problem 1: (12 Points) Describe the following concenpts in a concise way (focus on the most important things, no more than a couple sentences are needed)

- Fast Fourier Transform
- Multi-step methods
- Trapezoidal rule
- machine precision
- Givens rotation
- Cholesky decomposition

Problem 2: (4 Points) What is the relative condition number of addition when adding positive numbers?

Problem 3: (4 Points) Can you give a fixed point iteration for the solution of the equation

$$\frac{x}{2} + x^2 = \sin x? \tag{1}$$

(we are interested in the smallest positive root around $x = 0.5$). Does the proposed iteration converge?

Problem 4: (6 Points) Show that the iteration

$$x_{n+1} = \frac{2x_n}{3} + \frac{a}{3x_n^2} \tag{2}$$

converges to $\sqrt[3]{a}$ by showing that it's the Newton-Rhapson iteration for some function $f(x)$, the root of which is $\sqrt[3]{a}$.

Problem 5: (6 Points) When calculating a numerical derivative using the forward difference formula, what is the best stepsize that we can employ and why?

Problem 6: (6 Points) You have a matrix A and an approximate eigenvector $\mathbf{v}$. How can you calculate the corresponding eigenvalue? How can you improve the accuracy of $\mathbf{v}$ (such that it's closer to an exact eigenvector)?

Problem 7: (6 Points) Describe the Gradient descent method for finding minima of functions. Does it have a relation to the Newton-Rhapson method for root search? When does it find the global minima of a function?

Problem 8: (4 Points) Suppose you have a large matrix. How would you calculate its determinant? What is the cost of the method you propose?

Problem 9: (4 Points) Describe forward and backward substitution and explain when it might be needed when solving systems of linear equations.

Problem 10: (4 Points) You need to calculate an integral $\int_a^b f(x)dx$ where f(x) is some smooth function, and you are interested in the result to high accuracy. What method would you use and why? What method would you use, if you have $f(x)$ calculated from the numerical solution of a differential equation?

Problem 11: (6 Points) How can one calculate the eigenenergies of the one-dimensional Schrödinger equation with the potential

$$V(x) = \begin{cases} ax^2 & -L < x < L \\ \infty & x < -L \text{ or } x > L \end{cases}$$

numerically?