KFU Graz

Dénes Sexty (denes.sexty@uni-graz.at)

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)

- · Bisection method
- · rectangular rule
- · iterative solution of a system of linear equations
- The order of a method for solving ODEs
- · Aliasing in frequency analysis
- · Cholesky decomposition

Problem 2: (4 Points) Show that the relative condition number of substraction is infinity.

Problem 3: (8 Points) Describe the secant and the Newton-Rhapson method for the solution of a non-linear equation.

Problem 4: (6 Points) When calculating a numerical derivative using the central difference formula, what is the best stepsize that we can employ and why?

Problem 5: (4 Points) Suppose you have some datapoints x_i, y_i with $i = 1, \dots, 5$. What's the difference between a polynomial fit and a polynomial interpolation?

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 Golden ratio search for finding extrama of functions of one variable.

Problem 8: (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 9: (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 10: (6 Points) You have two datasets, a_i and b_i with $i = 1, \dots, N$. You need to calculate their convolution,

$$c_i = \sum_{k=1}^{N} a_k b_{i-k},$$

where you consider the datapoints to be periodic: $b_k = b_{N+k}$. How can you calculate c_i for $i = 1, \dots, N$ and what is the cost of the calculation?