KFU Graz
Dénes Sexty (denes.sexty@uni-graz.at)
Computational Physics WS 24-25

Example Exam

On the exam you will have similar questions (less of them such that there's enough time). You are allowed to use paper and pencil.

Problem 1: (10 Points) Describe the following concenpts in a concise way (focus on the most important things, no more than a couple sentences are needed)

- Multi-step methods
- Trapezoidal rule
- machine precision
- least squares fitting of a model function
- Gradient descent

Problem 2: (6 Points) When numerically searching for the root of an equation, under what conditions does the fixed-point iteration converge to a root of an equation? What can one do when it doesn't converge?

Problem 3: (6 Points) Show that the iteration

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

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 4: (6 Points) Show that the discretisation of the second derivative using the formula

$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

is correct up to corrections of $O(h^2)$. Calculate also the first correction term (proportional to h^2).

Problem 5: (6 Points) What algorithms do you know for calculating the inverse of a matrix? What is their cost?

Problem 6: (6 Points) Consider the matrix

$$A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Suppose you calculate its LU decomposition, then you can write $a_{11} = l_{11}u_{11}$ from which $u_{11} = 0$ follows, thus $\det A = \det LU = \det L \det U = \det U = 0$. What is wrong with the above reasoning? What do we do in practice when we want to LU decompose A?

Problem 7: (6 Points) Show that using the RK2 to solve the initial value problem $\dot{y} = f(y,t),\ y(0) = a$ with the stepsize $\Delta t \ll 1$, one should expect that we get $y(1)$ up to an error of $O(\Delta t^2)$.
(RK2: $y_{n+1} = y_n + hf\left(y_n + hf(y_n, t_n)/2, t_n + h/2\right)$)

Problem 8: (6 Points) You have two datasets, a_i and b_i with $i = 1, \cdots, N$. 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 $i = 1, \cdots, N$ and what is the cost of the calculation?

Problem 9: (6 Points) You are trying to solve the eigenvalue problem $y'''' - f(x)y = \lambda y,\ y(0) = y(1) = 0,\ y''(0) = y''(1) = 0$ numerically. Describe the steps of your solution using the shooting method.

Problem 10: (4 Points) Using the power algorithm on a matrix A, we calculate intermediate vectors $x_{p+1} = Ax_p$. Assuming that the algorithm converges, show that the eigenvalue of A corresponding to the converged vector can be estimated from

$$\lambda = \frac{x_{p+1}x_p}{x_p x_p}.$$