Practice questions

1. A derivate is calculated using the approximation

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

Assume that the roundoff error is $\sim \epsilon|f(x)|/h$. Estimate the lowest possible total error.

2. Derive a second-order Runge–Kutta method (i.e., third-order local error) for the problem $y'(x) = f(x, y)$, $y(0) = y_0$.

3. What is a stiff set of ordinary differential equations?

4. Give an example of a predictor–corrector method.

5. Describe Lagrange's interpolation formula.

6. Explain by an example what Richardson extrapolation is.

7. Describe the trapezoidal rule for integration. What is the form of the truncation error?

8. Explain Romberg's integration method.

9. Explain how the weights A_1, A_2 and abscissas x_1, x_2 are determined in the Gauss formula

$$\int_a^b f(x)w(x)dx \approx A_1 f(x_1) + A_2 f(x_2) .$$

For polynomials of what degree is the formula exact?

10. What is the definition of the Discrete Fourier Transform? Describe the general idea behind the Fast Fourier Transform. How do the computational costs scale with the number of sampling points for the Discrete and Fast Fourier Transforms?

11. Describe the Crank-Nicholson method for the one-dimensional heat equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \qquad 0 < x < 1 \qquad t > 0$$

with boundary conditions $u(0, t) = u_0$ and $u(1, t) = u_1$. Show that the method is stable.

12. A simple difference approximation of the equation $\partial u/\partial t = -v\partial u/\partial x$ is

$$\frac{u_j^{n+1} - u_j^n}{h} = -\frac{v}{2a}(u_{j+1}^n - u_{j-1}^n) , \tag{1}$$

where $u_j^n = u(x_j, t_n)$, $x_j = ja$, $t_n = nh$. Show that this method is unstable for all $h > 0$. Replacing u_j^n in (1) with $(u_{j+1}^n + u_{j-1}^n)/2$ gives the Lax method. What is the stability condition for the Lax method?

13. The Schrödinger equation

$$i\frac{\partial\psi}{\partial t} = -\frac{\partial^2\psi}{\partial x^2} + V(x)\psi$$

is to be solved numerically. Give an argument for the use of the Crank-Nicholson method.

14. Consider the Poisson equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -\rho(x,y) \qquad\qquad (x,y)\in\Omega$$

with boundary condition $u(x,y) = f(x,y)$, $(x,y)\in\partial\Omega$. Show that the solution to this problem minimizes

$$S[u] = \int_\Omega \left(\frac{1}{2}\nabla u\cdot\nabla u - \rho u\right) dxdy$$

(minimization over all functions $u = u_0 + \eta$, satisfying the boundary condition, u_o is the solution to the poisson equation and η is a function that is zero at the boundary).

Hint: Apply Gauss' theorem to $\eta\nabla u$ and show that

$$S[u_0+\eta] = S[u_0] + \frac{1}{2}\int_\Omega \nabla\eta\cdot\nabla\eta d^D x \tag{2}$$

15. Describe briefly Jacobi's method for the problem in the previous question. What is the difference between this method and the Gauss-Seidel method? How does the method of successive overrelaxation differ from the Gauss-Seidel method?

16. What is the definition of the characteristic function of a random variable X? How is it related to the probability distribution of X? What is a cumulant?

17. What does the central limit theorem say?

18. Explain how a random number with frequency function $p(x) = \lambda\exp(-\lambda x)$ for $x\geq 0$ and $p(x) = 0$ otherwise can be obtained from uniformly distributed random numbers.

19. Explain how a random number with frequency function $p(x) = \sqrt{2/\pi}\exp(-x^2/2)$ for $x\geq 0$ and $p(x) = 0$ otherwise can be obtained from uniformly distributed random numbers.

20. Suppose that one has access to n independent random numbers drawn from the distribution $p(x)$. Explain how these can be used to obtain an estimate I_n of the integral $I = \int f(x)p(x)dx$. Express the variance of I_n in terms of

$$\sigma_f^2 = \int f(x)^2 p(x)dx - \left(\int f(x)p(x)dx\right)^2.$$

21. What is meant by importance sampling?

22. Assume that $T_0, T_1, \ldots$ is a stationary Markov chain with transition probabilities $W(t\to t') = P\{T_{n+1} = t'|T_n = t\}$ (the state space is assumed to be discrete). Let $p_n(t)$ denote the distribution of T_n, i.e. $p_n(t) = P\{T_n = t\}$, and define the distance between two arbitrary distributions $p^{(a)}$ and $p^{(b)}$ by

$$||p^{(a)} - p^{(b)}|| = \sum_t |p^{(a)}(t) - p^{(b)}(t)|\,.$$

Show that if $p(t)$ is a stationary distribution, then $||p_{n+1} - p|| \leq ||p_n - p||$. Show also that this inequality is strict if $p_n \not\equiv p$ and $W(t\to t') > 0$ for all pairs t, t'.

23. What is meant by detailed balance? Show that detailed balance implies stationarity.

24. Explain how detailed balance is achieved in the Metropolis method.

25. What is meant by simulated annealing?

26. Newton's method for minimizing $f(\mathbf{x})$, $\mathbf{x} \in R^n$, is given by the recursion formula

$$\mathbf{x}' = \mathbf{x} - \mathbf{H} \cdot \nabla f(\mathbf{x}) \,,$$

where $\mathbf{H}$ denotes the inverse of the Hessian matrix, i.e. $(\mathbf{H}^{-1})_{ij} = \partial_i \partial_j f(\mathbf{x})$. Show that this method converges in one step if

$$f(\mathbf{x}) = c - \mathbf{b} \cdot \mathbf{x} + \frac{1}{2} \mathbf{x} \cdot \mathbf{A} \mathbf{x} \,, \tag{3}$$

where c is a number, $\mathbf{b}$ a vector and $\mathbf{A}$ a symmetric, positive definite matrix.

27. Minimizing $f(\mathbf{x})$, $\mathbf{x} \in R^n$, by successive line minimizations amounts to using a recursion formula of the form

$$\mathbf{x}_{i+1} = \mathbf{x}_i + \lambda_i \mathbf{h}_i \qquad i = 0, 1, \ldots$$

where the vector $\mathbf{h}_i$ gives the direction of the ith line and the number λ_i is determined by minimization.

   (a) Give an argument against the choice $\mathbf{h}_i = -\nabla f(\mathbf{x}_i)$ (steepest descent).

   (b) Show that if f has the form (3) and if $\mathbf{h}_{i-1}$ and $\mathbf{h}_i$ are conjugate ($\mathbf{h}_{i-1} \cdot \mathbf{A} \mathbf{h}_i = 0$), then $\nabla f(\mathbf{x}_{i+1}) \cdot \mathbf{h}_{i-1} = \nabla f(\mathbf{x}_i) \cdot \mathbf{h}_{i-1} = 0$.

28. Explain how the directions $\mathbf{h}_i$ (see previous question) are chosen in the conjugate-gradient method. What can be said about the convergence rate of this method if $f(\mathbf{x})$ is quadratic [see (3)]? Explain how the conjugate-gradient method can be used to solve linear systems of equations and what the advantage of this method is.