Practice/Oefen Exam: Deeltoets B

Question 1 (on lecture 1)

Consider the scalar field $g(x, y, z) = x^3z - 2y^2z^2$.

(a) Compute the gradient vector field $\mathbf{G} = \nabla g$.

(b) Calculate the divergence of the vector field $\mathbf{G}$, given by $\nabla \cdot \mathbf{G}$.

Question 2 (on lecture 2)

Consider the multivariable function $z = f(x, y) = 2x^2 + y^2 - 8x + 4y + 12$.

(a) Find the critical point (x_0, y_0) of $f(x, y)$.

(b) Construct the Hessian matrix H at this critical point and determine whether it corresponds to a local minimum, local maximum, or saddle point.

Question 3 (on lecture 3)

Consider a damped harmonic oscillator described by $\ddot{x} + 2\gamma\dot{x} + \omega_0^2 x = 0$.

(a) Formulate the system as two first-order ODEs for position x and velocity $v = \dot{x}$, and write down the update rule for x_{n+1} and v_{n+1} using the **Explicit Euler** method with time step Δt.

(b) Explain why the Explicit Euler method fails to conserve energy in un-damped physical systems ($\gamma = 0$) over long simulation times.

Question 4 (on lecture 4)

Solve the following second-order linear homogeneous differential equation with initial conditions:

$$y'' + 4y' + 4y = 0, \quad \text{with } y(0) = 3 \text{ and } y'(0) = -2.$$

Question 5 (on lecture 5)

Compute the continuous Fourier Transform $\hat{f}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t)e^{-i\omega t}dt$ of the asymmetric decaying exponential signal:

$$f(t) = \begin{cases} e^{-at}, & \text{if } t \geq 0, \\ 0, & \text{if } t < 0, \end{cases} \quad \text{where } a > 0.$$

Question 6 (on lecture 6)

Suppose we estimate a d-dimensional integral using either a multi-dimensional Simpson's rule (error scaling $\mathcal{O}(N^{-4/d})$) or Monte Carlo integration (error scaling $\mathcal{O}(N^{-1/2})$).

(a) Determine the critical dimension d^* above which Monte Carlo integration exhibits a higher rate of convergence than Simpson's rule.

(b) Briefly explain why Monte Carlo methods are preferred for molecular simulations involving $d = 300$ degrees of freedom.

Question 7 (on Lecture 7)

The rate of a first-order chemical reaction is modeled as $y = k \cdot t$, where y represents the log-concentration change, t is time (in seconds), and k is the reaction rate constant. The following data points were measured:

Time t (s)	1	2	4
Signal y	0.8	1.7	3.5

Formulate the linear system $Xk \approx \mathbf{y}$ and compute the optimal parameter k using the ordinary least squares formula $\hat{k} = (X^T X)^{-1} X^T \mathbf{y}$.