

Applied Math. and Computational Math. Individual (5 problems)

Problem 1. Consider the implicit leapfrog scheme

$$\frac{u_m^{n+1} - u_m^{n-1}}{2k} + a \left(1 + \frac{h^2}{6} \delta^2\right)^{-1} \delta_0 u_m^n = f_m^n$$

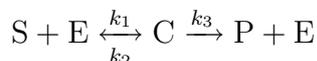
for the one-way wave equation

$$u_t + au_x = f.$$

Here δ^2 is the central second difference operator, and δ_0 is the central first difference operator.

- (1) show that the scheme is of order (2, 4).
- (2) show that the scheme is stable if and only if $|\frac{ak}{h}| < \frac{1}{\sqrt{3}}$.

Problem 2. A simple version of an enzyme-mediate chemical reaction process is given by



where S is the substrate reactant and P is the concentration of the desired product. An enzyme (or catalyst) E is a compound whose special property is that it allows for intermediate reaction steps that lead to the overall reaction,



Assume the initial conditions

$$S(0) = S_0, \quad E(0) = E_0, \quad C(0) = 0, \quad P(0) = 0;$$

k_1, k_2, k_3 are reaction rate constants.

- (a) Convert the chemical reaction equation into a system of rate equations (ODEs) for $S(T)$, $E(T)$, $C(T)$, and $P(T)$ where T is the dimensional time. Nondimensionalize the equations using the scalings

$$T = t/(k_1 E_0), \quad S(T) = S_0 s(t), \quad P(T) = S_0 p(t), \quad E(T) = E_0 e(t), \quad C(T) = E_0 c(t),$$

$$\epsilon = \frac{E_0}{S_0} \ll 1, \quad \lambda = \frac{k_2}{k_1 S_0}, \quad \mu = \frac{k_2 + k_3}{k_1 S_0}.$$

- (b) Use the expansions $s(t) = s_0(t) + \epsilon s_1(t) + O(\epsilon^2)$, $c(t) = c_0(t) + \epsilon c_1(t) + O(\epsilon^2)$, etc to determine the equations for the leading order slow solution. Show that $s_0(t)$ and $p_0(t)$ satisfies the following Michaelis-Menten equations

$$\dot{s}_0(t) = -(\mu - \lambda) \frac{s_0}{\mu + s_0}, \quad \dot{p}_0(t) = (\mu - \lambda) \frac{s_0}{\mu + s_0}.$$

Problem 3. We say that a vector $\mathbf{u} = (u_1, \dots, u_n) \in \mathbb{N}^n$ is *multiplicatively dependent* if there is a non-zero vector $\mathbf{k} = (k_1, \dots, k_n) \in \mathbb{Z}^n$ for which

$$(1) \quad u_1^{k_1} \cdots u_n^{k_n} = 1.$$

This notion plays a very important role in many number theoretic algorithms, such as *factorisation* and *primality testing*. It also (in a more general form) appears in some questions in *algebraic dynamics*. However the algorithm to decide whether \mathbf{u} is multiplicatively dependent is not immediately obvious. The following statement *informally* means that if \mathbf{u} is multiplicatively dependent the exponents k_1, \dots, k_n can be chosen to be reasonably small. Prove that if $\mathbf{u} = (u_1, \dots, u_n) \in \mathbb{N}^n$ is multiplicatively dependent with $\|\mathbf{u}\|_\infty \leq H$ where $\|\mathbf{u}\|_\infty = \max_{1 \leq i \leq n} |u_i|$, then there is a non-zero vector $\mathbf{k} = (k_1, \dots, k_n) \in \mathbb{Z}^n$ with

$$\|\mathbf{k}\|_\infty \leq \left(\frac{2n \log H}{\log 2} \right)^{n-1}$$

(and hence for a fixed n it can be found in polynomial time of order $(\log H)^{n(n-1)}$).

Comment: To solve this problem, you can use the following statement (without proof) which *informally* means that if a system of homogeneous equations with integer coefficients has a nontrivial solution then it has an integer solutions with reasonably small components. It is required in many applications.

Let $A = (a_{ij})_{i,j=1}^{m,n}$ be an $m \times n$ matrix of rank $r \leq n - 1$ with integer entries of size at most H , that is,

$$|a_{ij}| \leq H, \quad 1 \leq i \leq m, \quad 1 \leq j \leq n.$$

Then there is an integer **non-zero** vector $\mathbf{x} = (x_1, \dots, x_n) \in \mathbb{Z}^n$ such that $A\mathbf{x} = \mathbf{0}$ and

$$\|\mathbf{x}\|_\infty \leq (2nH)^{n-1}$$

where $\|\mathbf{x}\|_\infty = \max_{1 \leq i \leq n} |x_i|$.

Problem 4. Consider a symmetric matrix $A_{n \times n}$, and let λ_i be a simple eigenvalue of A with

$$|\lambda_j - \lambda_i| = O(1), \quad j \neq i.$$

In inverse iteration of compute eigenvalue and eigenvector, one needs to solve the following linear system

$$(A - \mu I)y_{k+1} = x_k,$$

where μ is an approximation of eigenvalue λ_i , $\|x_k\| = 1$ and obtain

$$x_{k+1} = \frac{y_{k+1}}{\|y_{k+1}\|}.$$

However, for μ close to λ_i , $A - \mu I$ has a very small eigenvalue and the linear system will be ill-conditioned. So there may be large error in the numerical solution to the linear system, denoted by \tilde{y}_{k+1} . Even though we may get large error in \tilde{y}_{k+1} , the \tilde{x}_{k+1} we get from $\tilde{x}_{k+1} = \frac{\tilde{y}_{k+1}}{\|\tilde{y}_{k+1}\|}$ is accurate.

(1) \tilde{y}_{k+1} satisfies

$$(A - \mu I + \delta A)\tilde{y}_{k+1} = x_k,$$

where $\|\delta A\| = O(\epsilon)$ and ϵ is the machine precision. Show that

$$(A - \lambda_i) \frac{\tilde{y}_{k+1}}{\|\tilde{y}_{k+1}\|} \leq |\mu - \lambda_i| + \|\delta A\| + \frac{1}{\|\tilde{y}_{k+1}\|}.$$

(2) Let $\alpha_i = x_k^t q_i$, where q_i is the normalized eigenvector corresponding to λ_i . Show that

$$\|\tilde{y}_{k+1}\| \geq \frac{|\alpha_i|}{|\mu - \lambda_i| + \|\delta A\|}.$$

(3) Conclude that

$$\|x_{k+1} - (\pm)q_i\| = O(|\lambda_i - \mu| + \epsilon).$$

Problem 5. A function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ in C^2 is called strongly convex if its Hessian matrix satisfies $\nabla^2 f \succeq mI$ for some $m > 0$. Show that the following statements are equivalent:

- (a) f is strongly convex, i.e. $\nabla^2 f(x) \succeq mI$ for all $x \in \mathbb{R}^n$;
- (b) For any $t \in [0, 1]$, any $x, y \in \mathbb{R}^n$,

$$f(tx + (1-t)y) \leq tf(x) + (1-t)f(y) - \frac{m}{2}t(1-t)\|x - y\|^2;$$

- (c) $\langle \nabla f(x) - \nabla f(y), x - y \rangle \geq m\|x - y\|^2$ for any $x, y \in \mathbb{R}^n$.