NATIONAL UNIVERSITY OF SINGAPORE

PC5215 – NUMERICAL RECIPES WITH APPLICATIONS

(Semester I: AY 2025-26)

Time Allowed: 2 Hours

INSTRUCTIONS TO STUDENTS

1. Write your student number on the answer book. Do not write your name.
2. This assessment paper contains FOUR questions and comprises THREE printed pages (including this cover page).
3. Students must answer ALL questions; each question carries equal marks.
4. Students should write the answers for each question on a new page.
5. This is a CLOSED BOOK examination.
6. Non-programable calculators are allowed.

1. This question concerns the LU decomposition of a square matrix.
   a. One way to perform the LU decomposition conveniently by hand is to use the right-looking recursive algorithm, which is given by the following steps: partition the matrix into sizes of 1 and $N-1$ blocks as
   $$\begin{bmatrix} a_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \text{ and transform it into } \begin{bmatrix} a_{11} & A_{12} \\ l & \tilde{A}_{22} \end{bmatrix},$$
   where $l = A_{21}/a_{11}$ and $\tilde{A}_{22} = A_{22} - lA_{12}$. Note that l is a column vector of $(N-1)$ by 1, while A_{12} is a row vector of 1 by $(N-1)$, the resulting outer product lA_{12} is an $(N-1)$ by $(N-1)$ square matrix. Apply the steps recursively to the smaller subblock $\tilde{A}_{22}$. Finish in $N-1$ steps. Given the following matrix
   $$A = \begin{bmatrix} 1 & 2 & -2 \\ 1 & 0 & -1 \\ 2 & -1 & 3 \end{bmatrix},$$
   work out the LU decomposition using the recursive method.
   b. Compute the determinant of the matrix A, using the result in part a.
   c. Based on the description in part a, what is the computational complexity of this algorithm?

a) During the first step, the 2 by 2 block $A_{22} = \begin{bmatrix} 0 & -1 \\ -1 & 3 \end{bmatrix}$ *is transformed into* $\tilde{A}_{22} = \begin{bmatrix} 0 & -1 \\ -1 & 3 \end{bmatrix} - \begin{bmatrix} 1 \\ 2 \end{bmatrix} [2 \quad -2] = \begin{bmatrix} -2 & 1 \\ -5 & 7 \end{bmatrix}$. *Applying the rule recursively, in the second step, this 2 x 2 block is transformed to* $\begin{bmatrix} -2 & 1 \\ \frac{5}{2} & \frac{9}{2} \end{bmatrix}$ *(here now* $l = 5/2$ *and* $\tilde{A}_{12} = 1$ *are 1 by 1 matrix). So the final matrix is transformed into* $\begin{bmatrix} 1 & 2 & -2 \\ 1 & -2 & 1 \\ 2 & \frac{5}{2} & \frac{9}{2} \end{bmatrix}$ *where the upper triangular part including the diagonal is U, and the strict lower triangular part with 1 on the diagonals implied is L. i.e. LU are in the place of original A, just like in the Crout algorithm. b) det(A) = det(U) = -9. c) the computational complexity is* $O(N^3)$*. We need scan through the smaller matrices N-1 times,* $(N-1)^2 + (N-2)^2 + .. 1^2 \approx N^3$.

2. In a Markov chain Monte Carlo method, we consider the following transition matrix,
$$W = \begin{bmatrix} 0 & 1 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{bmatrix}$$

   Answer the following questions:

   a. Is the Markov chain ergodic, and why?
   b. Determine the invariant (or equilibrium) distribution P such that $P = PW$. Here, P is a row vector.

c. State the detailed balance equation.
d. Does the above Markov chain, defined by the transition matrix W, satisfy detailed balance?

Yes, it is ergodic as it is irreducible (every state can be reached from any other state in three steps), and it is aperiodic (because the diagonal W(3,3) is not zero). Also, since W^3> 0 for all i, j. b) solve the equation P = PW, with normalization, P(1) + P(2) +P(3) = 1, we find P = (3/10, 4/10, 3/10). c The detailed balance means P(i) W(i -> j) = P(j) W(j -> i), for all i and j. d. No, we can check with i = 1, j = 2, for example. P(1)W(1->2) = 3/10 x 1 = 3/10, while P(2) W(2->1) = 4/10 x 1/2 = 2/10. So it does not satisfy the detailed balance equation.

3. Consider the following function of a generic quadratic form

$$f(x) = \frac{1}{2} x^T A x - b^T x + c.$$

Here x and b are column vectors of dimension N, A is an $N \times N$ symmetric, positive definite matrix, and c is just a number. Answer the following questions:

a. What is the gradient $g = \nabla f$ of the function f at point x?
b. What is the Hessian matrix of the function f at point x?
c. Suppose we are at a point x_0 and want to move to the minimum using the Newton iteration method. How should the value x be updated, and in how many steps?
d. If instead, the conjugate gradient is used, then how should it be updated, and in how many steps can the minimum be reached?

We can use the fact $\frac{\partial}{\partial x} x^T = I$, I is the identity matrix, or directly work in component form, so a) the gradient is $g = \nabla f = Ax - b$, and b) the Hessian matrix is $H = \nabla\nabla f = A$ (or use the component form $\frac{\partial^2 f}{\partial x_i \partial x_j} = A_{ij}$). c) The Newton iteration is $x_1 = x_0 - H^{-1} \nabla f|_{x_0} = x_0 - A^{-1}(Ax_0 - b) = A^{-1} b$. This means, we get to the minimum in one step, as the gradient now is 0. The Newton iteration is much faster than the steepest descent. d) For the conjugate gradient, the new search direction is $n' = -g' + \gamma n$, where $\gamma = |g'|^2/|g|^2$ here n is the previous search direction for the line search, n' is the current search direction, g' is the current gradient, and g is the previous gradient. Line search means we find the minimum of $f(x + \lambda n)$ with respect to λ. It takes exactly N steps to reach the minimum in N dimensions.

4. The one-dimensional diffusion equation for the density n of gas particles is similar to the Schrödinger equation, only all the quantities are real, given by

$$\frac{\partial n(x,t)}{\partial t} = D \frac{\partial^2 n(x,t)}{\partial x^2}.$$

Here we consider the problem as defined in all space $x \in (-\infty, +\infty)$ evolving in time t. D is the diffusion constant. The total number of particles $N(t) = \int_{-\infty}^{+\infty} n(x,t)dx$ is finite.

a. Show analytically that $\frac{dN(t)}{dt} = 0$, using the diffusion equation. This means the total number of particles is a constant.
b. We solve the diffusion equation numerically by finite difference. Give a discretization scheme to approximate the time-development using the implicit Euler method, meaning that the time derivative is approximated by backward difference, at time t and $t - h$, while the second derivative in space is approximated by central difference at time t at discrete locations $x = ja$. Here j is an integer, and a is the spatial spacing.
c. Show, by summing over the space points j, the total number of particles, $N(t) = a\sum_j n(ja, t)$, is conserved according to the equation in part b.
d. Rewrite the discrete equation in part b as a matrix equation $An = b$. Here the column vector n has the elements $n_j = n(ja, t)$. Identify the matrix A and the right-hand vector b. How could you solve this equation and what is the best computational complexity per step?

Note $\frac{dN}{dt} = \int_{-\infty}^{+\infty} \frac{\partial n(x,t)}{\partial t} dx$, i.e., we can move the time derivative inside the integral but then it becomes partial derivative. Using the diffusion equation, $\int_{-\infty}^{+\infty} \frac{\partial^2 n}{\partial x^2} dx = \left.\frac{\partial n}{\partial x}\right|_{-\infty}^{+\infty}$ and the fact that the density at infinity is zero, we obtain dN/dt = 0. b) the backward Euler algorithm is $n(x,t) - n(x, t-h) = \frac{Dh}{a^2}\,[n(x+a,t) - 2n(x,t) + n(x-a,t)]$. c) sum over j with discretization $x = ja$, j runs from minus infinity to plus infinity as integers, we find $N(t) - N(t-h) = \frac{Dh}{a^2}\big(N(t) - 2N(t) + N(t)\big) = 0$, so the number of particle number N is conserved exactly. d) in matrix form, A is tridiagonal with diagonal value $1 + 2\alpha$, and first off-diagonals with $-\alpha$ (each row or column sum to 0), here $\alpha = Dh/a^2$. That is $A = \begin{bmatrix} 1+2\alpha & -\alpha & 0 \\ -\alpha & 1+2\alpha & -\alpha \\ 0 & -\alpha & 1+2\alpha \end{bmatrix}$. The tri-diagonal linear system $An = b$ can be solved in $O(N)$, just like for the last homework for the Schrodinger equation. Here the right-hand side b is n at the previous step.

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