NATIONAL UNIVERSITY OF SINGAPORE

PC5215 – NUMERICAL RECIPES WITH APPLICATIONS

(Semester I: AY 2018-19)

Time Allowed: 2 Hours

INSTRUCTIONS TO STUDENTS

1. Please write your student number only. Do not write your name.
2. This assessment paper contains FIVE questions and comprises TWO printed pages.
3. Students are required to answer ALL questions; questions carry equal marks.
4. Students should write the answers for each question on a new page.
5. This is a CLOSED BOOK examination.
6. Non-programmable calculators are allowed.

1. Given a matrix A, if we perform an LU decomposition without pivoting, the process may fail. Consider $A = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & -1 \\ 1 & 0 & -1 & 0 \end{bmatrix}$. Make a LU decomposition with pivoting (swap rows), and specify how you have permuted the matrix, such that $PA = LU$.

The answer depends on how we permute the rows. If we permute 1 ↔ 2, and 3 ↔ 4, then $P = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$, $L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix}$, $U = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & -2 \end{bmatrix}$. *The permutation needed can be found by trial and error, or you start with the Crout's algorithm. But when it fails, you can go back to permute the rows. The final result can be checked to see if PA = LU.*

2. Consider Gaussian quadrature on the whole real line $(-\infty, +\infty)$ with an Gaussian weight, $\int_{-\infty}^{+\infty} f(x)e^{-\frac{x^2}{2}}dx = \sum_{i=1}^{N} w_i f(x_i)$.
   a. Determine the first three orthogonal polynomials, P_0, P_1, and P_2.
   b. Give the two-point Gaussian quadrature formula, i.e., $N = 2$.

a. The first three orthogonal polynomials are of the form, $P_0 = c$, $P_1 = ax+b$, $P_2 = ax^2 + bx + c$. Without loss of generality, we can choose the coefficients of the highest power to be 1. So $P_0 = 1$. P_1 need to be orthogonal to P_0, so we need the integral of $(ax+b)\exp(-x^2/2)dx = 0$. Noting odd function integrates to 0, we must have $b = 0$. So $P_1 = x$. Lastly, P_2 also need to be orthogonal to P_0 and P_1. Again using the fact that odd function integrates to 0, and the Gaussian integrals (with x^2 multiplied or not) give values $\sqrt{2\pi}$, we find $a + c = 0$. Finally, P_1 is orthogonal to P_2, we find $b = 0$, and $P_2 = x^2 - 1$. Note: using Hermite or Legendre polynomial is not correct, as the weight function is different.

b. With N = 2, x_1 and x_2 are determined by the roots of P_2, giving $x_1 = -1$, $x_2 = +1$. w_1 and w_2 are determined if we set $f(x) = 1$ or x, which gives the value of the integral $\sqrt{2\pi}$ or 0. So $w_1 = w_2 = \sqrt{\pi/2}$.

3. The Metropolis algorithm in Monte Carlo method can be used to generate arbitrary complex distribution for random variables.
   a. State the Metropolis algorithm.
   b. Apply this algorithm to generate a random variable x with the distribution $p(x) = (2 - x)/2,\ 0 \le x < 2$, and 0 otherwise. Give your answer in terms of pseudo code.
   c. What is your choice of move in terms of the transmission matrix $T(x \to x')$?

a. *Use a single real variable x as an example (but Metropolis algorithm is very general), we start off by setting x to some arbitrary value. Then we propose a move x' = x + δ where δ is small random variable centered around 0 within some window uniformly distributed. [It is not wrong to let x' be a uniformly distributed random number between 0 and 2, i.e., x' = 2 ξ, completely independent of x. But this is not the usual Metropolis]. We then compute the ratio p(x')/p(x), set r = min(1, p(x')/p(x)). The new value x' is accepted with probability r (rejected with probability 1-r). This is repeated sufficiently large number of N times. Then the distribution of x will be p(x).*
b. *Pseudo code is omitted here. One implements it by drawing two random numbers in each step, one for the choice of δ, and one for comparison with r. Note that the function p(x) should be defined properly such that when x < 0 or x > 2, p(x) = 0. So that x could not getting a value outside the validity region 0 < x < 2.*
c. *T(x->x') represents the proposal move x' -> x + δ, which is a uniform distribution centered around x, within a window [x-Δ/2, x+Δ/2], if we set δ = (0.5 – ξ)Δ, where ξ uniformly distributed random number between 0 and 1. Note that T(x->x') appears in the total transition matrix as, W(x->x') = T(x->x') min(1, p(x')/p(x)).*

4. Consider a square matrix A of dimension $N \times N$ multiplying a column vector x of dimension $N \times 1$, giving a new column vector $b = Ax$.
    a. What is the computational complexity of a matrix multiplying a vector?
    b. Let's assume the matrix A has periodicity, i.e., $A_{ij} = A((i-j) \bmod N)$, demonstrate that now $b = Ax$ can be computed faster using fast Fourier transform (FFT). Outline the steps. What is the new computational complexity?

a. *Each element of b is obtained by a scalar product of a row of A with the column vector x, which takes O(N). We need to do this N times. The overall computational complexity is $O(N^2)$.*
b. *Due to the periodicity in A, we can write the problem as a discrete convolution. We fast Fourier transform the vector x into y, and Fourier transform the vector A (as a function of one index, A(i)), to B. Multiplying the two vectors, elementwise y(k)B(k) for each k, and then inverse transform the result back, we obtain b. This takes O(N log N), because of the use of fast Fourier transform.*

5. Consider the Schrödinger equation $i\hbar \frac{\partial \Psi}{\partial t} = \widehat{H}\Psi$.
    a. Working in one-spatial dimension with coordinate x, show that the wave-function normalization is a conserved quantity, i.e., $\frac{d}{dt}\int |\Psi|^2 dx = 0$.
    b. Consider numerical solution of the time-dependent Schrödinger equation with the Euler method of a time step h. Show explicitly that the wave-function normalization is violated. Work out an error estimate, i.e., define $c(t) = \int |\Psi(t,x)|^2 dx$, then set $c(t+h) = c(t) + O(h^N)$, find the integer N.

c. Show that the Trotter-Suzuki operator splitting method preserves normalization exactly.

a. *If we use the inner product or Dirac notation, $(\Phi,\psi) = \langle\Phi|\psi\rangle$, the normalization is just $(\psi,\psi)=1$. Using the fact that the operator $\hat{H}$ is hermitian, i.e., $(\hat{H}\Phi, \psi) = (\Phi, \hat{H}\psi)$, the proof is immediate. Without using this notation, and assuming the usual Hamiltonian, $\hat{H}=-(\hbar^2/2m)d^2/dx^2+V(x)$, in 1D, we need to do integrations by part two times to shift the x derivative from the first term to the second term, in order for the two kinetic energy terms, $\psi^* (H\psi)$ and $(H\psi)^* \psi$ to get cancelled. Note that ψ is not an eigenstate of $\hat{H}$, so we cannot use $\hat{H}\psi=E\psi$, and ψ in general is complex. Thus, the derivatives to ψ and to its complex conjugate are not equal.*

b. *The Euler method is to take $\psi(t+h) = \psi(t) – (i/\hbar)\, h\, \hat{H}\psi(t)$. The normalization of $\psi(t+h)$ got a cross term linear in h, which is 0 if we assume $\psi(t)$ is normalized, as proved in part a. So the error in $c(t+h)$ is $O(h^2)$.*

c. *In Trotter-Suzuki, $\exp(-ihT/\hbar)\exp(-ihV/\hbar)$, each step is to multiple a pure phase factors to the wave function (in x space or momentum p space). The normalization is obtained by taking modulus $|\psi(x)|^2$ (or similarly the wave function in p space representation), then sum over x (or p). Clearly, a phase factor does not change the modulus squared. Normalization is maintained for both the potential energy step and kinetic energy step. Or alternatively, each of the steps is strictly a unitary transformation to the wave function.*

--the end-- WJS