**NATIONAL UNIVERSITY OF SINGAPORE**

PC5215 – NUMERICAL RECIPES WITH APPLICATIONS

(Semester I: AY 2017-18)

Time Allowed: 2 Hours

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## 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. Answer briefly the following short questions/concepts.
   (a) What is a machine epsilon? Give the numerical value of the machine epsilon associated with the IEEE double precision.
   (b) What is the time computational complexity of computing a matrix inverse, $A^{-1}$, of an $N \times N$ matrix? Explain why.
   (c) What is a symplectic algorithm in molecular dynamics? Give an example of such an algorithm for solving numerically the harmonic oscillator problem, $H = \frac{p^2}{2m} + \frac{1}{2}kx^2$.
   (d) Define what is a heap in the heap sort method.

*(a) The machine ε is such that the next larger number than 1 that is representable in a floating point format is 1+ε. For IEEE double precision, the next value is $1 + 2^{-52}$=1.000…1 (52 bit for mantissa), so the machine $\epsilon = 2^{-52} \approx 2.2 \times 10^{-16}$.*

*(b) Computational complexity for taken matrix inverse is $O(N^3)$, why? Same as solving linear equation. LU decomposition takes $N^3$, then forward/backward substitution N times.*

*(c) Numerical algorithm for the Hamiltonian system that preserve the two-form, $\sum_i dp_i \wedge dq_I$ exactly, or in other words, the transformation from one step to next is a canonical transformation. For the harmonic oscillator, we can use $p_{n+1} = p_n - kx_n dt, x_{n+1} = x_n + p_{n+1} dt/m$ .*

*(d) Heap is a binary tree such that the value at the parent node is not smaller than the children nodes.*

2. Bode's rule is one of the closed Newton-Cotes formula involving five equally spaced points, $x_i = ih$, $i = 1,2, \ldots ,5$, as follows: $\int_{x_1}^{x_5} f(x)dx = (\alpha f_1 + \beta f_2 + \gamma f_3 + \beta f_4 + \alpha f_5)h + O(h^n)$. Notice that the coefficients are symmetric. (a) Consider polynomials of the form, $1, x, x^2, \ldots$ , up to what degree of the polynomials Bode's rule is exact? (b) based on part (a) determine a set of linear equations for the three coefficients $\alpha, \beta, \gamma$. No need to solve them. (c) What is the power $n$ in the error estimate $O(h^n)$.

*(a) Up to $x^5$, this is due to the extra symmetry of the formula.*

*(b) It is more convenient to shift the origin to $x_3$, so that we have $x_1$=-2h, $x_2$=-h, $x_3$=0, x4=h, $x_3$=2h, then the equations are for even power, f(x)=1, $4 = 2\alpha + 2\beta + \gamma$, $for\ f(x) = x^2, \frac{16}{3} = 8\alpha + 2\beta$, and for $f(x) = x^4, \frac{32}{5} = 16\alpha + \beta$. For odd power f = x, $x^3$, $x^5$, it produces 0=0 identity due to symmetry.*

*(c) n=7.*

3. (a) State what is an LU decomposition. (b) Consider the linear equations determined in part 2(b), perform the LU decomposition without using pivot. (c) Obtain the solution for $\alpha, \beta, \gamma$, using forward substitution, followed by backward substitution.

*(a) write A as A = LU where L is lower triangular with diagonals set to 1, U is upper triangular.*
*(b) The form of A is not unique, as long as A = LU, and Ax=b, it is considered correct. For example,*

$A = \begin{pmatrix} 2 & 2 & 1 \\ 4 & 1 & 0 \\ 16 & 1 & 0 \end{pmatrix}, L = \begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 8 & 5 & 1 \end{pmatrix}, U = \begin{pmatrix} 2 & 2 & 1 \\ 0 & -3 & -2 \\ 0 & 0 & 2 \end{pmatrix}$,

*Then for* $b = \begin{pmatrix} 4 \\ 8/3 \\ 32/5 \end{pmatrix}$, *we get* $\alpha = \frac{14}{45}, \beta = \frac{64}{45}, \gamma = \frac{8}{15}$.

4. We consider Monte Carlo simulation for light propagation. An isotropic point light source is located at Cartesian coordinate (0,0,*d*). (a) Let $\xi_i$ be given uniformly distributed random numbers in the interval [0,1) for $i = 1, 2, 3, \cdots$. Give a method to generate a random ray emitting from (0,0,*d*) with uniform distribution in a sphere centered around (0,0,*d*). (b) Suppose the ray generated in part (a) hits a diffusive surface at $z$=0 at some point (*x*, *y*,0). Then the ray is randomly reflected off the surface, uniformly distributed in the upper half space about the plane. Using the random numbers given in (a), determine the equation for the outgoing ray.

   (a) *We write the outgoing ray in the vector form* $\mathbf{r} = \mathbf{r}_0 + \mathbf{n}\, t$, *then the 3D unit vector* $\mathbf{n}$ = $(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, *with* $\phi = 2\pi\xi_1, \theta = \arccos(1 - 2\xi_2)$. *Uniform distribution on a sphere implies* $P(\theta,\phi)d\Omega = \frac{d\Omega}{4\pi}$, *where* $d\Omega = \sin\theta\, d\theta d\phi$ *is the solid angle.*
   (b) *Same, except we restrict t z>0, or* $0 < \theta < \frac{\pi}{2}$.

5. Consider the conjugate gradient (CG) method for the solution of the minimum of a quadratic form $f(x) = \frac{1}{2}x^T Ax - b^T x$, here $x$ is a column vector of dimension $N$, and $A$ is a matrix of $N \times N$. (a) What conditions one must impose to $A$ in order for the CG method to work? (b) Consider a specific matrix $A$ and $b$ as follows: $A = \begin{bmatrix} 4 & -2 & 0 \\ -2 & 2 & 1 \\ 0 & 1 & 4 \end{bmatrix}$, $b = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$. Set $x_0 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$, determine the search direction $d_0$ and residue $r_0$. Note the first search direction is the negative gradient direction. (c) Determine $d_1$ and $r_1$ and show explicitly $d_0^T A d_1 = 0$ and $r_0^T r_1 = 0$.

   (a) *CG method need A symmetric and positive definite.*
   (b) *The first search direction is the negative gradient,* $d_0=r_0=b-Ax_0 = (-3,2,-1)^T$.
   (c) *We stop at* $x_1=x_0+\alpha d_0 = (13/34,7/17,-7/34)^T$. *here* $\alpha = |r_0|^2/(d_0^T Ad^0)=7/34$. *So the residue* $r_1=b-Ax_1 =(5/17,5/34,-10/17)^T$. *From this we find orthogonality* $r_0^T r_1=0$. *New search direction is* $d_1=r_1+\gamma d_0 = (455/2312, 245/1156, -1435/2312)$. $\gamma=|r_1|^2/|r_0|^2=75/2312$. *Then we can check that the conjugate condition is true,* $d_0^T Ad_1 = 0$.

\- The end - [WJS]