NATIONAL UNIVERSITY OF SINGAPORE

PC5215 – NUMERICAL RECIPES WITH APPLICATIONS

(Semester I: AY 2014-15)

Time Allowed: 2 Hours

INSTRUCTIONS TO CANDIDATES

1. Please write your student number only.
2. This examination paper contains FIVE questions and comprises THREE printed pages.
3. Answer ALL the questions; questions carry equal marks.
4. Answers to the questions are to be written in the answer books.
5. Please start each question on a new page.
6. This is a CLOSED BOOK assessment.
7. Non-programmable calculators are allowed.

1. Answer briefly the following questions and concepts.
   a. What is the *time* computational complexity and *space* (memory) computational complexity of the LU decomposition algorithm of Crout?
   b. Give the mathematical definition of the norm $\| x \|$ of a vector in a linear space.
   c. What is a heap as used in data sorting?
   d. Explain the main concept of conjugate gradient method and answer why the minimum can be located in a finite number of *N* steps. What is the meaning of *N*?

a. The time computational complexity of an LU decomposition of a square matrix is $O(N^3)$, while space (memory) complexity is $O(N^2)$, where N is the dimension of the square matrix. Some students forget to say what is N.

b. The norm $||x||$ of a vector x in a linear space is a real number that must satisfy: positivity $||x|| \geq 0$, equal sign occurs only for zero vector $x=0$; scaling $||\alpha x|| = |\alpha| \, ||x||$, and triangle inequality $||x+y|| \leq ||x|| + ||y||$. Many students only give specific examples, (e.g., Euclidean 2-norm), but we need a general definition.

c. Heap is a binary tree arranged such that a parent node is not less than the two children. This forms a partial order.

d. The key idea in the conjugate gradient method is to take the search direction u_i such that $u^T_i A u_j = 0$ if $i \neq j$, called A-orthogonal. In this way the search stops in N steps where N is the dimensionality of the matrix A, and the function to minimize is of the quadratic form $f=(1/2)\, x^T A\, x - b^T x + c$. Many students give the algorithm without mentioning the important point of A-orthogonality.

2. Consider an IEEE-like floating point representation with a 16-bit word size. The highest bit denotes the sign (0 bit for positive number and 1 bit for negative number). The next 5 bits are used for a biased exponent *e*. All values *e* = 0, 1, 2, …, 31 will be used to represent a floating point number, without special types (such as NaN, or ∞). The rest of 10 bits will be used for the fractional part.
   a. What bias one should use so that both large and small number in magnitude as compared to 1 can be represented similar to the standard IEEE 754?
   b. What is the machine epsilon of this representation?
   c. What are the largest and smallest values in absolute magnitude in this representation?
   d. What is the number of significant figures in decimal for a typical 16-bit floating-point number?

a. Since the 5 bits for the exponent takes values from 0 to 31, we take bias = 15, half way from 0 to 31.

b. Machine epsilon $\varepsilon = 2^{-10} = 1/1024 \approx 0.001$.

c. *Largest value 1.11…1 × 216 =$(2\text{-}2^{-10})\times 2^{16}$ = 131008, smallest value $2^{-15} \approx 3.05\times 10^{-5}$.*
d. *Based on $\varepsilon \approx 0.001$, the number of significant figures are 3 in decimal.*

If bias is choosing to be 16, the values change slightly accordingly.

3. In a closed Newton-Cotes integration formula of N points, polynomials of degrees $N-1$ is integrated exactly without error.
   a. Determine the coefficients α_i in a three-point integration formula $\int_0^{2h} f(x)dx = \alpha_0 f_0 + \alpha_1 f_1 + \alpha_2 f_2 + O(h^?)$, where $f_i = f(ih)$.
   b. By coincidence or otherwise, show that polynomials of degree 3 also integrate exactly by the above formula.
   c. Based on the derivation in part a and b, deduce the order of error of the integration formula.

a. *We set the function f(x) to be 1, x, and x^2, evaluating the left and right side of the equation, obtain, $2h = \alpha_0 + \alpha_1 + \alpha_2$; $(2h)^2/2 = \alpha_0\, 0 + \alpha_1 h + \alpha_2 2h$; and $(2h)^3/3 = \alpha_0\, 0 + \alpha_1 h^2 + \alpha_2 (2h)^2$. Solving the linear equations, one finds the Simpson's rule, $\alpha_0 = h/3$, $\alpha_1 = 4h/3$, and $\alpha_2 = h/3$.*
b. *Set $f(x) = x^3$, we find left-hand side ($4h^4$) equals right-hand side. Since the formula is linear, this is sufficient to illustrate that it holds for general polynomials of degree 3.*
c. *Since it is accurate to $O(h^4)$ by part b, the error has to be of order h^5.*

Some students try to do Gaussian quadrature and determine the orthogonal polynomials, which is irrelevant here for this problem. Others try to do Taylor expansions.

4. Consider a three-spin system with the energy $H = -J(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_1 + \sigma_1\sigma_2\sigma_3)$, where $J > 0$, $\sigma_i = \pm 1$, $i = 1,2,3$. Assume a single-spin flip dynamics, i.e., a site i is chosen at random with equal probability.
   a. Determine the transition matrix W at temperature T.
   b. What is the left eigenvector p with eigenvalue $\lambda = 1$, i.e., $p = pW$?
   c. Outline the pseudo-code to perform Metropolis Monte Carlo calculation of the total heat capacity C, using the Markov chain specified exactly as in part a by W.

a. *The energies of each of the states are*

label	*Spin configuration*	*Energy E(i)*
1	+++	–4J
2	++–	2J
3	+–+	2J
4	–++	2J
5	––+	0

6	$+--$	*0*
7	$-+-$	*0*
8	$---$	*–2J*

Using the order given above, the transition matrix W is

$$\begin{bmatrix} 1-z & \frac{z}{3} & \frac{z}{3} & \frac{z}{3} & 0 & 0 & 0 & 0 \\ \frac{1}{3} & 0 & 0 & 0 & 0 & \frac{1}{3} & \frac{1}{3} & 0 \\ \frac{1}{3} & 0 & 0 & 0 & \frac{1}{3} & \frac{1}{3} & 0 & 0 \\ \frac{1}{3} & 0 & 0 & 0 & \frac{1}{3} & 0 & \frac{1}{3} & 0 \\ 0 & 0 & \frac{y}{3} & \frac{y}{3} & \frac{2-2y}{3} & 0 & 0 & \frac{1}{3} \\ 0 & \frac{y}{3} & \frac{y}{3} & 0 & 0 & \frac{2-2y}{3} & 0 & \frac{1}{3} \\ 0 & \frac{y}{3} & 0 & \frac{y}{3} & 0 & 0 & \frac{2-2y}{3} & \frac{1}{3} \\ 0 & 0 & 0 & 0 & \frac{y}{3} & \frac{y}{3} & \frac{y}{3} & 1-y \end{bmatrix}$$

Where $z = y^3$, $y = \exp(-2J/(k_B T))$.

b. *By construction, the equilibrium distribution is canonical,* $P(i) \propto \exp(-E(i)/(k_B T))$, *so* $P = (1/Z)\times(\exp(\beta 4J), \exp(-\beta 2J), \exp(-\beta 2J), \exp(-\beta 2J), 1, 1, 1, \exp(\beta 2J))$, *partition function* $Z = \exp(\beta 4J) + 3\exp(-\beta 2J) + 3 + \exp(\beta 2J)$. $\beta = 1/(k_B T)$. *There is no need to solve the linear equation, P = PW, explicitly.*

c. *E=0, C=0;*

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Do m = 1 to 10^6 {
  i = floor( 1 + 3ξ1);
  compute ΔE = E(new) – E(old);
  if( ξ2 < exp(-βΔE)) {
     σi = - –σi;
     }
   E = E + E(i);
   C = C + E(i)^2;
};
C = (1/10^6) { C – (E/10^6)^2 }/(kB T^2)
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Where E(new) means the energy with spin i flipped. E(i) is the energy recomputed after the Monte Carlo move. Some students forgot the formula for heat capacity, which is in our lab 3.

5. We prove the Trotter-Suzuki formula and use it to derive a symplectic integration scheme for a Hamiltonian system.
    a. The standard Trotter-Suzuki formula takes the form $e^{\varepsilon(\hat{A}+\hat{B})} = e^{\varepsilon\hat{A}}e^{\varepsilon\hat{B}} + O(\varepsilon^2)$ where $\hat{A}$ and $\hat{B}$ are non-commuting operators in some linear space, and ε is small. Prove this formula and show explicitly that the error is second order in the small quantity ε.
    b. Consider a mechanical system with the Hamiltonian $H(p,q)$ of a one degree of freedom with the coordinate q and conjugate momentum p. Then the equation of motion is $\dot{F} = -\{H,F\} = -\hat{\hat{L}}_H F$, where the curly bracket is the Poisson bracket, $\{H,F\} = \frac{\partial H}{\partial q}\frac{\partial F}{\partial p} - \frac{\partial F}{\partial q}\frac{\partial H}{\partial p}$, $\hat{\hat{L}}_H$ is the Liouvillian operator defined above by the Poisson bracket. Show that we can write the time-dependent solution of an arbitrary function of q and p formally in the form $F(t) = e^{-t\hat{\hat{L}}_H}F(0)$.
    c. Derive a symplectic algorithm for $H = \frac{p^2}{2m} + V(q)$, using the Trotter-Suzuki formula derived in part a, identifying the operator $\hat{A}$ and $\hat{B}$ with the kinetic energy term, $\frac{p^2}{2m}$, and potential energy term $V(q)$, respectively, in the Liouvillian.

    a. *Taylor expand both sides, multiply through (taken care of noncommuting nature of the operator), we find* $e^{\varepsilon(\hat{A}+\hat{B})} - e^{\varepsilon\hat{A}}e^{\varepsilon\hat{B}} = \frac{\varepsilon^2}{2}\left(\hat{B}\hat{A} - \hat{A}\hat{B}\right) + \cdots$.
    b. *Take time derivative to the solution,* $F(t) = e^{-t\hat{\hat{L}}_H}F(0)$, we find $d\frac{F(t)}{dt} = -\hat{\hat{L}}_H e^{-t\hat{\hat{L}}_H}F(0) = -\hat{\hat{L}}_H F(t)$. Some students try to solve the differential equation as if $\hat{\hat{L}}_H$ is a number, which is wrong. $\hat{\hat{L}}_H$ *is operator acting on functions.*
    c. *Using the formal solution and Trotter-Suzuki formula, we have* $F(t) = e^{-t\hat{\hat{L}}_H}F(0) \approx e^{-t\hat{\hat{L}}_T}e^{-t\hat{\hat{L}}_V} F(0)$. *Take F to be the vector (p,q), we obtain,*
    $$\begin{pmatrix} p_1 \\ q_1 \end{pmatrix} = e^{-t\hat{\hat{L}}_T}\begin{pmatrix} p_{1/2} \\ q_{1/2} \end{pmatrix}, \quad \begin{pmatrix} p_{1/2} \\ q_{1/2} \end{pmatrix} = e^{-t\hat{\hat{L}}_V}\begin{pmatrix} p_0 \\ q_0 \end{pmatrix}$$
    The explicit form can be found by Taylor expanding the exponentials, and use the definition of double hats and Poisson brackets, we find
    $$q_{1/2} = q_0, \quad p_{1/2} = p_0 + t\, f_0$$
    $$q_1 = q_{1/2} + t\, p_{1/2}/m, \quad p_1 = p_{1/2}$$

--- the end --- [WJS]