**NATIONAL UNIVERSITY OF SINGAPORE**

PC5215 – NUMERICAL RECIPES WITH APPLICATIONS

(Semester I: AY 2012-13)

Time Allowed: 2 Hours

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## INSTRUCTIONS TO CANDIDATES

1. This examination paper contains FIVE questions and comprises THREE printed pages.
2. Answer ALL the questions; questions carry equal marks.
3. Answers to the questions are to be written in the answer books.
4. This is a CLOSED BOOK examination.
5. Non-programmable calculators are allowed.

1. The IEEE 754 standard for floating point representation of the double precision number has a sign bit, followed by 11 bits for the biased exponent (with a bias of 1023) and the rest 52 bits for the fractional part.
    a. Give the bit patterns for the 64-bit double precision representation of −1 and 1/3.
    b. Discuss what impact reducing the biased exponent field to 8 bits has, in terms of the precision and magnitude of the floating point numbers.

*a. -1 is (in hexadecimal notation) BFF FFFFFFFFFFFFF,*
*1/3 is 3FD 5555555555555.*
*b . If the exponent field is reduced and fractional part increased, then the precision increases (machine epsilon is smaller) but the magnitude decreases.*

2. Consider numerical integration formula by Gaussian quadrature method.
    a. State the main idea of Gaussian quadrature.
    b. Consider a three-point Gaussian quadrature formula in the interval [0,1], $\int_0^1 f(x)dx \approx w_1 f(x_1) + w_2 f(x_2) + w_3 f(x_3)$. For polynomials, 1, $x$, $x^2$, …, $x^n$, the formula is exact. What is the largest integer $n$ that this is true?
    c. Determine the three-point formula, i.e., determine the abscissas $x_1$, $x_2$, $x_3$, and the weights $w_1$, $w_2$, $w_3$.

*a . by changing both the weights and abscissas, a maximum of accuracy is obtained, i.e., the formula is exact for polynomials of order 2N-1 for N point Gaussian quadrature.*
*b. n=5.*
*c.* $P_0 = 1$, $P_1 = x-1/2$, $P_2=x^2-x+1/6$, $P_3=x^3-3/2x^2+3/5x -1/20$. *This is obtained by the orthogonal condition* $\langle P_i|P_j\rangle = 0$ *(i < j). The root of* $P_3(x)=0$ *gives* $x_1=1/2$, $x_2 = (1-\sqrt{3/5})/2$, $x_2 = (1+\sqrt{3/5})/2$. *The weights are determined by the condition that the polynomials 1, x,* $x^2$ *can be integrated exactly. Given,*

$$\begin{cases} w_1+w_2+w_3=1, \\ x_1w_1+x_2w_2+x_3w_3=\dfrac{1}{2}, \\ x_1^2w_1+x_2^2w_2+x_3^2w_3=\dfrac{1}{3}. \end{cases}$$

*The solution is* $w_1=4/9$, $w_2=w_3=5/18$.

3. Consider a Monte Carlo simulation to generate Boltzmann distribution using the Metropolis algorithm for the following statistical-mechanical model:

$$H(\{\sigma_1,\sigma_2,\sigma_3\}) = -J\sigma_1\sigma_2 - J\sigma_2\sigma_3 - J(\sigma_1+\sigma_3),$$

where the spins $\sigma_i = \pm 1, i = 1,2,3$, and $J>0$ is some constant.

   a. Assuming that the spins are chosen at random with equal probability, determine the transition matrix *W*.
   b. What is the equilibrium/invariant distribution *P* associated with *W*?
   c. Outline pseudo-code that computes $\langle \sigma_1 \rangle$, i.e., the equilibrium average value of the first spin, in a Metropolis Monte Carlo simulation.

*a. The energy of the 8 states are*

| | | |
|---|---|---|
| 1 | + + + | $-4J$ |
| 2 | + + − | 0 |
| 3 | − + + | 0 |
| 4 | + − + | 0 |
| 5 | − + − | $+4J$ |
| 6 | + − − | 0 |
| 7 | − − + | 0 |
| 8 | − − − | 0 |

*The transition matrix is (in the same order as the state/energy list above)*

$$\begin{bmatrix} 1-3r & r & r & r & 0 & 0 & 0 & 0 \\ 1/3 & 1/3-r & 0 & 0 & r & 1/3 & 0 & 0 \\ 1/3 & 0 & 1/3-r & 0 & r & 0 & 1/3 & 0 \\ 1/3 & 0 & 0 & 0 & 0 & 1/3 & 1/3 & 0 \\ 0 & 1/3 & 1/3 & 0 & 0 & 0 & 0 & 1/3 \\ 0 & 1/3 & 0 & 1/3 & 0 & 0 & 0 & 1/3 \\ 0 & 0 & 1/3 & 1/3 & 0 & 0 & 0 & 1/3 \\ 0 & 0 & 0 & 0 & r & 1/3 & 1/3 & 1/3-r \end{bmatrix}, \qquad r = \frac{1}{3}e^{-4J/(kT)} .$$

b . *By design, P is the equilibrium (canonical) distribution, P =exp(-H(σ)/kT)/Z, ie., P = [exp(4J/kT), 1, 1, 1, exp(-4J/kT), 1, 1, 1]/Z, Z = 6 + exp(-4J/kT) + exp(4J/kT), satisfies P=PW (But we don't need to solve the eigenvalue problem to get P, as the purpose of the Metropolis algorithm is to design W such that P is the equilibrium one).*

*c . set $\sigma_1=\sigma_2=\sigma_3=1$. M=0.*

*for(i=1 to $10^6$) {*

*j = floor(3ξ) + 1,*

*Compute H(σ),*

*$\sigma_j = -\sigma_j$,*

*compute again $H(\sigma')$ (where the spin j is flipped), $\Delta E = H(\sigma')-H(\sigma)$,*

*if ($\xi_2 > \exp(-\Delta E/(kT))$) {*

*$\sigma_j = -\sigma_j$, (flip back)*

*},*

*$M = M + \sigma_1$,*

*}*

*$M = M/10^6$.*

4. The algorithm of the conjugate-gradient method for locating minimum is as follows:
   i. Initialize $\mathbf{n}_0 = \mathbf{g}_0 = -\nabla f(\mathbf{x}_0)$, $i = 0$,
   ii. Find $\lambda$ that minimizes $f(\mathbf{x}_i+\lambda\mathbf{n}_i)$, let $\mathbf{x}_{i+1} = \mathbf{x}_i+\lambda\mathbf{n}_i$
   iii. Compute new negative gradient $\mathbf{g}_{i+1} = -\nabla f(\mathbf{x}_{i+1})$
   iv. Compute $\gamma_i = \dfrac{\mathbf{g}_{i+1}\cdot\mathbf{g}_{i+1}}{\mathbf{g}_i\cdot\mathbf{g}_i}$
   v. Update new search direction as $\mathbf{n}_{i+1} = \mathbf{g}_{i+1} + \gamma_i\mathbf{n}_i$; $++i$, go to ii

   a. If $f$ is a function of two scalar variables $x$ and $y$,

   $$f = \frac{1}{2}x^2 + xy + y^2 - x + y,$$

   how many times do we need to iterate the steps?

   b. Starting from the point $(x,y)=(0,0)$, determine $\mathbf{n}_0$ and $\mathbf{n}_1$ according to the algorithm above and show that $\mathbf{n}_0^T A\, \mathbf{n}_1=0$, where $A$ is the coefficient matrix of the quadratic term in $f$.

   c. Work out the steps to find the minimum $(x_{\min}, y_{\min})$ of $f$.

*a . in two steps since it is two dimensional.*

*b . $n_0 = g_0 = (-x-y+1,-(x+2y+1)) = (1, -1)$,*

*$f = (1/2)\lambda^2 - 2\lambda$, min is at $\lambda=2$, $(x_1, y_1) = (2,-2)$, $g_1=(1,1)$,*

*$\gamma = 1$, $n_1 = (1,1) + \gamma(1,-1) = (2, 0)$.*

$$A = \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix},\ n_0^T A\, n_1 = 0.$$

*c . $(x_2,y_2) = (3,-2)$ is the minimum location.*

5. Consider the problem of damped nonlinear oscillator governed by the second order differential equation,

$$\frac{d^2x}{dt^2} = -\gamma \frac{dx}{dt} - x^3 + F(t),$$

where $\gamma$ is a damping constant and $F(t)$ some external driving force which depends on time explicitly.

a. Rewrite the equation as a set of first order differential equations equivalent to the original one.
b. Give the numerical algorithm of the midpoint method, and determine the local truncation error, i.e., the order $n$ in error $O(h^n)$ where $h$ is step size.
c. Give a version of symplectic algorithm, if possible. If not possible, explain why not?

*a* .
$$\begin{cases} \frac{dx}{dt} = y, \\ \frac{dy}{dt} = -\gamma y - x^3 + F(t). \end{cases}$$

*b . the midpoint algorithm is, in general:*

$$\mathbf{K}_1 = h\mathbf{F}(t, \mathbf{Y}_n)$$
$$\mathbf{K}_2 = h\mathbf{F}(t_n + \frac{h}{2}, \mathbf{Y}_n + \frac{\mathbf{K}_1}{2})$$
$$\mathbf{Y}_{n+1} = \mathbf{Y}_n + \mathbf{K}_2 + O(h^3)$$

*where errors are of $3^{rd}$ order, and vectors are*

$$\mathbf{Y} = \begin{bmatrix} x \\ y \end{bmatrix}, \quad \mathbf{F}(t, x, y) = \begin{bmatrix} y \\ -\gamma y - x^3 + F(t) \end{bmatrix}$$

*In component form for this problem, we have*

$$x_{n+1} = x_n + h\left( y_n + \frac{h}{2}(-\gamma y_n + x_n{}^3 + F(t_n) \right)$$
$$y_{n+1} = y_n + h\left[ -\gamma\left( y_n + \frac{h}{2}(-\gamma y_n + x_n{}^3 + F(t_n) \right) + (x_n + \frac{h}{2} y_n)^3 + F(t_n + \frac{h}{2}) \right]$$

*c . No, since the system cannot be derived from a Hamiltonian due to the damping or time-dependent forces. [It has nothing to do with linear or nonlinear].*

[JSW]

\- the end -