National University of Singapore

CZ5101 – NUMERICAL RECIPES

(Semester I: AY 2008-09)

26 Nov 2008 – Time Allowed: 2 hours

Instructions to Candidates:

1. This is a closed book examination.
2. This examination paper contains FIVE (5) questions and comprises FOUR (4) printed pages.
3. Each question carries 25 marks.
4. Answer any FOUR (4) questions.
5. Calculators are allowed.

1. Answer briefly the following questions:

    a. The IEEE 754 has representations for the special number $+\infty$ and $-\infty$. Give the bit patterns of the 32-bit floating point plus and minus infinities. Explain with one example that such numbers are useful.

    b. Prove that $F^* F = IN$, where F denotes the $N\times N$ matrix for the standard discrete Fourier transform, H = F h, in matrix notation; h and H are column vectors of length N. I is the identity matrix. What is the algorithmic complexity of a fast Fourier transform?

    c. A function passes through exactly the point (0,0), (1,0), (2,2), (3,0), where the first number is the independent variable x, the second number the value y. Give the unique polynomial that interpolates the four points.

    d. Consider a set of measured values 1.02, 1.10, 0.97, 1.01 for a quantity x. Estimate the average of x and the error on the average from the observational data.

a. $+\infty$*: 0 11111111 00000000000000000000000*
$-\infty$*: 1 11111111 00000000000000000000000*
usage, e.g., 1/(+∞) = 0.0

b. $F_{jk} = e^{i2\pi jk/N}$.

$$(F^*F)_{jk} = \sum_l F^*_{jl}F_{lk} = \sum_{l=0}^{N-1} e^{i2\pi(k-j)l/N}$$
$$= \frac{1-e^{i2\pi(k-j)}}{1-e^{i2\pi(k-j)/N}} = \begin{cases} 0, & \text{if } k \neq j \\ N, & \text{if } k = j \end{cases}$$

The computational complexity is O(N log N).

c. $$y(x) = \frac{x(x-1)(x-3)}{(2-0)(2-1)(2-3)} \cdot 2 = -x^3 + 4x^2 - 3x.$$

d.
$$\langle x \rangle = \frac{1}{4}(1.02 + 1.10 + 0.97 + 1.01) = 1.025,$$
$$\langle x^2 \rangle = \frac{1}{4}(1.02^2 + 1.10^2 + 0.97^2 + 1.01^2) = 1.05285,$$
$$\text{error in } \langle x \rangle = \sqrt{\frac{\langle x^2 \rangle - \langle x \rangle^2}{4-1}} = 0.0272,$$
or we report as $1.025 \pm 0.027.$

2. Consider Gaussian quadrature in the interval (0, +∞) with an exponential weight e^{-x}.

   a. Determine the first three monic polynomials $P_n(x)$ of degree 0, 1, and 2, such that $\int_0^{+\infty} e^{-x} P_n(x) P_m(x) dx \propto \delta_{nm}$. You may use the integration formula $\int_0^{+\infty} x^n e^{-x} dx = n!$.

   b. Determine the weights and abscissas of (i) a one-point Gaussian quadrature formula and (ii) a two-point Gaussian quadrature formula. Write out the formulas explicitly.

   c. For what sort of functions $g(x)$ the two-point Gaussian quadrature formula is exact for the integration $\int_0^{+\infty} g(x)\, dx$?

a. Choose $P_0(x)=1$, let $P_1(x)=x+c$, such that $\int_0^{\infty} P_0(x) P_1(x) e^{-x} dx = \int_0^{\infty} (x+c) e^{-x} dx = 0$.
This gives $c = -1$, i.e. $P_1(x)=x-1$. Similarly, let $P_2(x)=x^2+bx+c$, and make it orthogonal to P_0 and P_1, we find $P_2(x)=x^2-4x+2$.

b. For one point formula, x is solution of P_1, weight is determined by $\int_0^{\infty} f(x) e^{-x} dx = wf(1)$ *for f = const. We find w = 1. For two point formula, the abscissas are the solutions of $P_2(x)=0$. so* $x_1 = 2-\sqrt{2}, x_2 = 2+\sqrt{2}$. *The weights are determined by* $\int_0^{\infty} f(x) e^{-x} dx = w_1 f(x_1) + w_2 f(x_2)$ *for $f(x)=1$, and $f(x)=x$. or*
$\int_0^{\infty} e^{-x} dx = w_1 + w_2 = 1$, $\int_0^{\infty} x e^{-x} dx = w_1 x_1 + w_2 x_2 = 1$. *The solutions are*
$w_1 = \frac{2+\sqrt{2}}{4}, w_2 = \frac{2-\sqrt{2}}{4}$.

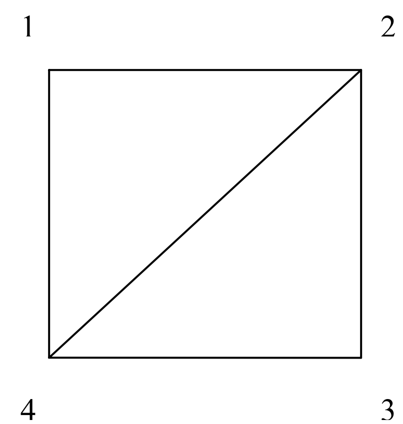
c. The formula is exact for $g(x)=p(x)e^{-x}$, where $p(x)$ is a polynomial of degree 0, 1, 2, and 3.

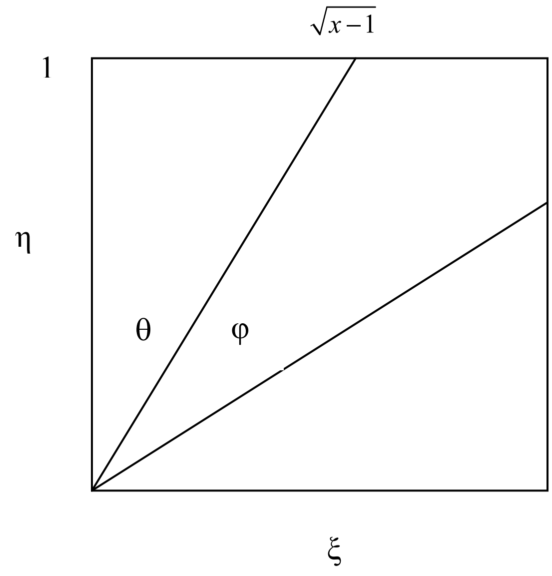
3. Consider the following problems in Monte Carlo methods.

   a. Two variables ξ and η are independent, uniformly distributed random numbers from 0 to 1. Determine the probability density $p(x)$ of the new random variable $x = \xi^2 + \eta^2$.

   b. Consider a particle diffusing among the corners 1, 2, 3, 4 of a square, as shown below. If the particle is at position 1 or 3, the particle moves with equal probability to its neighbor 2 or 4 in the next step. If the particle is at positions 2 or 4, it moves with 1/3 probability to its neighbors or its diagonal.

      i. Give the transition matrix of the Markov chain associated with the random walk.
      ii. Give the equation for the invariant (equilibrium) probability distribution of the Markov chain and solve it numerically.





a. *The cumulative distribution is* $F(x) = P(\xi^2 + \eta^2 < x) = \int_{\substack{0<\xi<1,\,0<\eta<1,\\ \xi^2+\eta^2<x}} d\xi d\eta$. *The integration represents the common area of a quad circle of radius* $\sqrt{x}$ *with the unit square. There are 4 cases. If x < 0, the integral is 0; if x > 2, the integral is 1. If x < 1, it is just the area of ¼ of a circle of radius* $\sqrt{x}$. *The most difficult case is when 1 < x < 2, which can be calculated geometrically as the sum of two right-angle triangles with sides 1 by* $\sqrt{x-1}$, *plus the area of circle section extending an angle φ=π/2-2θ, where tan θ=* $\sqrt{x-1}$ *(or cosθ=1/*$\sqrt{x}$ *). See the figure above. So we have*

$$F(x) = \begin{cases} 0, & x < 0 \\ \pi x/4, & 0 < x < 1 \\ \sqrt{x-1} + x(\frac{\pi}{4} - \tan^{-1}\sqrt{x-1}), & 1 < x < 2 \\ 1, & x > 2 \end{cases}$$

The probability is obtained by differentiation, P(x)=dF(x)/dx.

b. *(i) The transition matrix W is*

$$\begin{pmatrix} 0 & \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{3} \\ 0 & \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 \end{pmatrix}.$$

(ii) The equilibrium distribution satisfies $P^T W = P^T$, or in components,

$$p_1 = \frac{1}{3}p_2 + \frac{1}{3}p_4,$$
$$p_2 = \frac{1}{2}p_1 + \frac{1}{2}p_3 + \frac{1}{3}p_4,$$
$$p_3 = \frac{1}{3}p_2 + \frac{1}{3}p_4,$$
$$p_4 = \frac{1}{2}p_1 + \frac{1}{3}p_2 + \frac{1}{2}p_3.$$

Notice the symmetry that $p_1 = p_3$, $p_2 = p_4$, the solution is found to be $p_1 = 1/5$, $p_2 = 3/10$.

4. Consider the theory of conjugate gradient method for iteratively solving the system of linear equations

   $$Ax = b \quad \text{with} \quad A = A^T.$$

   The solution of the above equation can be reformulated as to find the minimum of a quadratic form $f(x)$.

   a. Give the expression of the quadratic form f.
   b. Consider two arbitrary vectors d_0 and d_1 as search directions. Determine conditions such that f is minimized for line searches, with starting point x_0, in the direction d_0, stopping at x_1, and then in the direction d_1, stopping at x_2. Give the form of x_1 and x_2 in terms of the starting point, search direction, matrix A, and vector b.
   c. Consider the same two vectors d_0 and d_1. Determine conditions such that f is minimized at x' in the two-dimensional plane spanned by the two vectors containing the starting point x_0.
   d. Determine a condition on the search directions d_0 and d_1 such that performing part b or c obtains equivalent results, i.e., determine the condition that $x_2 = x'$.

a. $f = \frac{1}{2}x^T A x - b^T x$.

b. Let $x = x_0 + \lambda d_0$, the minimum x_1 in the direction d_0 is obtained from
$\frac{\partial f}{\partial \lambda} = d_0^T \nabla f_{|x} = d_0^T(Ax - b) = d_0^T(Ax_0 + \lambda A d_0 - b) = 0$. *$\lambda$ is solved to be* $\lambda_0 = \frac{d_0^T(b - Ax_0)}{d_0^T A d_0}$,
and $x_1 = x_0 + \lambda_0 d_0$. Similarly, $x_2 = x_1 + \lambda_1 d_1$, with $\lambda_1 = \frac{d_1^T(b - Ax_1)}{d_1^T A d_1}$.

c. Let $x' = x_0 + \lambda_0 d_0 + \lambda_1 d_1$. x' is determined by two coupled linear equations for λ_0 and λ_1 given by $\frac{\partial f}{\partial \lambda_0} = 0, \frac{\partial f}{\partial \lambda_1} = 0$. *Or*

$$d_0^T Ax = d_0^T (Ax_0 - b + \lambda_0 Ad_0 + \lambda_1 Ad_1) = 0,$$
$$d_1^T Ax = d_1^T (Ax_1^{'} + \lambda_1 Ad_1) = d_1^T (Ax_0 - b + \lambda_0 Ad_0 + \lambda_1 Ad_1) = 0.$$

d. If $d_0^T Ad_1 = 0$*, equations in part c becomes the same as that in part b. If* $x_2=x'$*, we must demand this A-orthogonal condition for search directions.*

5. Consider the following linear least squares problem.

   a. The minimization of the sum of weighted χ-square errors
   $$\sum_{j=1}^{N} \frac{1}{\sigma_j^2}(y_j - a\,x_j - b)^2$$
   in linear least squares problem leads to a normal equation, where σ_j is the standard deviation in the data y_j, and a and b are fitting parameters. Let the normal equation be of the form
   $$C\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \end{bmatrix}.$$
   Give the corresponding matrix elements c_{ij} and d_i of the normal equation for the above minimization problem.

   b. The errors of the fitting parameters can be also computed, assuming an independent Gaussian noise for the errors of y_j. Derive the formula for the error of the slope a.

   c. Explain briefly the meaning of "goodness-of-fit".

a.
$$c_{11} = \sum_j \frac{x_j^2}{\sigma_j^2}, \quad c_{12} = c_{21} = \sum_j \frac{x_j}{\sigma_j^2}, \quad c_{22} = \sum_j \frac{1}{\sigma_j^2},$$
$$d_1 = \sum_j \frac{x_j y_j}{\sigma_j^2}, \quad d_2 = \sum_j \frac{y_j}{\sigma_j^2}.$$

b. The solution of a is
$$a = \frac{\begin{vmatrix} d_1 & c_{12} \\ d_2 & c_{22} \end{vmatrix}}{\begin{vmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{vmatrix}} = \frac{d_1 c_{22} - d_2 c_{12}}{D} = \frac{1}{D}\left[c_{22}\left(\sum_j \frac{x_j y_j}{\sigma_j^2}\right) - c_{12}\left(\sum_j \frac{y_j}{\sigma_j^2}\right)\right].$$
$$= \sum_j \frac{c_{22} x_j - c_{12}}{D\sigma_j^2} y_j$$

Using the formula for variance, we get (note that x and c, D are constants)

$$\begin{aligned}\sigma_a^2 = \mathrm{var}(a) &= \sum_j \left(\frac{c_{22}x_j - c_{12}}{D\sigma_j^2}\right)^2 \mathrm{var}(y_j) \\ &= \sum_j \frac{c_{22}^2 x_j^2 - 2c_{12}c_{22}x_j + c_{12}^2}{D^2\sigma_j^4}\sigma_j^2 = \frac{c_{22}^2 c_{11} - 2c_{22}c_{12}^2 + c_{12}^2 c_{22}}{D^2} \\ &= \frac{c_{22}}{D}.\end{aligned}$$

c. *Goodness-of-fit is the probability that the χ^2 value is equal or large than the observed value. If this probability is too small or to close to 1, the fitting is not good.*

See also the NR textbook, Chap 15.2.

– **the End** –

[JSW]