National University of Singapore

PC5215 – NUMERICAL RECIPES WITH APPLICATIONS

(Semester I: AY 2011-12)

Time Allowed: 2 hours

Instructions to Candidates:

1. This examination paper contains FOUR questions and comprises THREE printed pages.
2. This is a closed book examination.
3. Questions carry equal marks.
4. Answer all FOUR questions.
5. Non-programmable calculators are allowed.

1. Answer briefly the following questions:
   a. Is there a difference in the programming language C when a fixed size array or a pointer is passed to a function, like int a[10], or int *a, in sub(a)?
   b. Explain the meanings of catastrophic cancellation and benign cancellation, respectively, in numerical arithmetic.
   c. What is the main idea of Gaussian quadrature? Give the one-point Gaussian quadrature formula in the interval [0,1] with weight of 1.
   d. How accurately can one locate with a single precision number (float in C) a minimum using a typical search algorithm (e.g., bisection)?

a. There is no difference in C for passing array or pointer to a function.

b. Catastrophic cancelation means a great loss of accuracy (e.g. all significant figures are lost) in a numerical arithmetic; benign cancelation means some accuracy is still maintained (e.g., accuracy is reduced by half).

c. In Gaussian quadrature, both the weight and abscissa (x value) are allowed to adjust in order to achieve maximum accuracy respect to the integration of a polynomial. For a one point formula, we require that the values are exact for 1 and x, this fixes the weight and w=1, and x_0=1/2., i.e., $\int_0^1 f(x)dx = f(1/2)$.

d. The relative accuracy in a search algorithm is $\sqrt{\varepsilon}$. *For single precision, it is about 4 significant figures.*

2. Consider matrices of A, B, C, D of dimensions $N \times N$, $N \times M$, $M \times N$, and $M \times M$, respectively. Using these matrices, we can do a block matrix LU decomposition of the form (assuming A^{-1} exists):

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} I_N & 0 \\ \alpha_{21} & I_M \end{pmatrix} \begin{pmatrix} \beta_{11} & \beta_{12} \\ 0 & \beta_{22} \end{pmatrix},$$

where I_N and I_M are identity matrices of size N and M, respectively, and α and β are matrices of suitable sizes.

   a. Find the matrices α and β in terms of matrices A, B, C, D. Pay attention to the order as matrices do not commute in general.
   b. Using the result in a, express the determinant of the matrix $\begin{pmatrix} A & B \\ C & D \end{pmatrix}$ of dimension $(N+M) \times (N+M)$ in terms of a product of determinants of two smaller matrices of sizes $N \times N$ and $M \times M$.

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} I_N & 0 \\ CA^{-1} & I_M \end{pmatrix} \begin{pmatrix} A & B \\ 0 & D - CA^{-1}B \end{pmatrix}$$

$$\det\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \det(A)\det(D - CA^{-1}B)$$

3. Consider the Metropolis algorithm of Markov chain Monte Carlo simulation applied to Ising spin systems.
   a. A single spin $\sigma = \pm 1$ in a magnetic field h (>0) is made in contact with a thermal heat bath such that the equilibrium distribution is given by the Boltzmann distribution $\exp(-H/(k_B T)]/Z$ at temperature T with a Hamiltonian $H = - h\,\sigma$. Since there is only one spin, in a Metropolis algorithm we always choose it and flip it according to the standard Metropolis rate. Give the 2×2 transition matrix W_a.
   b. Now repeat the above problem for a two-spin system with a new Hamiltonian (energy function) as $H = - J\, \sigma_1\sigma_2$, (J>0). For this purpose, give a 4×4 matrix W_b describing the Markov chain of the Metropolis algorithm, where each spin is choosen with equal probability.
   c. What is the stationary (equilibrium) distribution P of the transition matrix W_b in part b? Justify your answer.

a. Assuming the first is +, second -, then $W_a = \begin{pmatrix} 1-x & x \\ 1 & 0 \end{pmatrix}, \quad x = e^{-2h/(k_B T)}$.

b. Assuming matrix entries in the order ++, +-, -+, and - -, then

$$W_b = \begin{pmatrix} 1-r & \frac{r}{2} & \frac{r}{2} & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 0 & \frac{r}{2} & \frac{r}{2} & 1-r \end{pmatrix}, \qquad r = e^{-2J/(k_B T)}$$

c. $P \propto e^{-H/(k_B T)} \propto (1, r, r, 1)$. *P is the stationary distribution. This can be verified directly or solved by PW = P.*

4. In the conjugate gradient (CG) method for determining the minimum of a quadratic function, one starts from some point moving in the steepest descent direction to a local minimum in that direction, and then move in a new direction $\mathbf{n}_{i+1} = \mathbf{g}_{i+1} + \gamma \mathbf{n}_i$, where γ is

the ratio of the magnitude squared of the gradient of present step to the previous step, $\gamma = \mathbf{g}_{i+1} \cdot \mathbf{g}_{i+1} / \mathbf{g}_i \cdot \mathbf{g}_i$. Consider the following function in three variables *x*, *y*, *z*.

$$f(x,y,z) = \frac{1}{2}\left[(x-1)^2 + 2y^2 + \frac{1}{2} z^2 \right].$$

a. How many steps at most will it take for the CG method to converge to the answer?
b. What is the expected minimum location (*x*,*y*,*z*) without going through the CG steps?
c. Following the CG steps exactly as in the algorithm, find the minimum of the function, starting from (0,1,1) [Use of calculator is encouraged].

a. 3 steps as the problem is in three dimensions.

b. x=1, y=0, z=0, obtained by setting the partial derivatives to 0.

c. The steps are, given x_0=(0,1,1), compute g_0=n_0=(-x+1,-2y,-z/2)=(1,-2,-1/2). Minimized $f(\lambda)=f(x_0+\lambda n_0)$, obtain λ = 0.57534, obtain new $x_1 = x_0 + \lambda n_0$, and obtain $\gamma=|g_1|^2/|g_0|^2$=0.0758116, and obtain new $n_1 = g_1+\gamma n_0$, etc. We list the values in a table for the three steps:

(x,y,z)	*g*	*n*	*λ*	*γ*
(0,1,1)	*(1,-2,-0.5)*	*(1,-2,-0.5)*	*0.575342*	*0.0758116*
(0.5753, -0.1506, 0.712)	*(0.424, 0.301,-0.356)*	*(0.5004,0.1497,-0.394)*	*1.06716*	*0.084399*
(1.109, 0.0091, 0.2917)	*(-0.109,-0.0182,-0.145)*	*(-0.067,-0.00559,-0.17915)*	*1.62871*	
(1,0,0)				

[WJS]

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