NATIONAL UNIVERSITY OF SINGAPORE

PC5215 – NUMERICAL RECIPES WITH APPLICATIONS

(Semester I: AY 2015-16)

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. The IEEE 754 single precision floating-point format has one sign bit at the most significant position, followed by 8-bit for the biased exponent with a bias of 127, followed by 23-bit for the fractional part (mantissa).
    a. Consider the following binary calculation of the floating point values, z = x + y, where x = 0011 1110 1000 0000 0000 0000 0000 0000,
    y = 1011 1110 0111 1111 1111 1101 0110 0001.
    Determine z as bit pattern.
    b. Determine the absolute errors in x and y due to finite representation of real numbers in floating-point format. Determine the error in the result z, and give the number of significant figures in z (number of meaningful figures in decimal not counting leading zeros).

    a) The numerical value of x is 0.25, and y is -0.24999, but we don't need to know. The important point is that when adding/subtracting, the exponent of one of them must shifted so that they have the same exponent, the result is z = 0 0110 1110 010 011110xxx… The xxx means whose digits we don't know and it is part of the error in z.

    b) Absolute errors are 1.5×10^{-8}, and 7×10^{-9}, 3×10^{-8}, for x, y, z, respectively. The number of significant figures of z is at most 9 in binary and 3 in decimal. Due to the closeness of x and $|y|$, subtraction causes a great loss of accuracy.

2. Páde approximation is similar to polynomial interpolation except that it is given by the ratio of two polynomials, for example,
$$e^x = 1 + x + \frac{x^2}{2} + \cdots \approx \frac{c_0+c_1x+\cdots+c_Nx^N}{1+d_1x+\cdots d_Mx^M}.$$
    a. Determine the coefficients of the right-hand side when $N = M = 1$.
    b. Give a general method (algorithm) to determine the coefficients c_i and d_j.

    Hint: multiply the denominator to the left-side, and match the coefficients of the polynomials.

    a) The answer is exp(x) ≈ (1+x/2)/(1-x/2). b) We have N+M+1 unknowns. We need form sufficient equations to determine them uniquely, so the expansion should not stop, but up to $x^{(N+M)}$ with the power larger than N set to 0. See also NR book Chap.3.2, Chap.5.12.

3. The following pseudo C code is written for a Monte Carlo simulation of the one-dimensional Ising model with the Hamiltonian $H(\sigma) = -J\sum_{i=1}^{N}\sigma_i\,\sigma_{i+1}$, with periodic boundary condition, e.g., $\sigma_{N+1} = \sigma_1$. Based on the code, determine the transition matrix W of the Markov chain and its equilibrium distribution p, such that $p = pW$.

    i = a random integer from 1 to *N*;
    $\Delta = (2J/k_B\,T)\,(\sigma_{i-1} + \sigma_{i+1})$;
    $r = e^{-\Delta}/(1 + e^{-\Delta})$;

σ_i= sign(ξ - *r*);

where k_B is the Boltzmann constant, *T* is temperature, *J* > 0 is the ferromagnetic coupling constant, ξ is a uniformly distributed random number from 0 to 1, and *i*, Δ, and *r* are temporary variables. sign(*x*) is the sign function taken value 1 if *x* > 0 and -1 otherwise.

The program says that we set the spin up (+1) with probability 1-r, and down (-1) with probability r. This means we don't care about the value of the spins before flip so it is not Metropolis. The transition matrix W (which is a 2^N by 2^N matrix) consists of two parts, the part T(σ->σ') which denotes the selection of the spins at random, so T is 1/N if two states differ by one spin, and zero otherwise. The rate part is (fixing all other spins and focus only on site i, $\begin{pmatrix} 1-r & r \\ 1-r & r \end{pmatrix}$, where entries are ordered according to +, -. Since 1-r is the conditional probability of being +, given the values of all other spins, and r is the conditional probability of being -, if the overall probability is the canonical distribution, it is clear $(\sigma) = \exp\big(-\beta H(\sigma)\big)/Z$ *. This method of Monte Carlo simulation is known as heat-bath algorithm, or Gibbs sampler.*

4. Consider the problem of fitting a curve with the exponential form $f(x) = Ae^{-kx}$. By working with the natural logarithm of the function $\ln f$, instead of f, we can turn a nonlinear fit to a linear least-squares fit. Let (x_i, y_i) be the set of data points for x and f, with standard deviation in f as σ_i (assuming small), $i = 1,2,\cdots N$.
   a. Derive formulas for the parameters A and k.
   b. Determine the errors (one standard deviation) in A and k.

   Hint: The standard least-squares formulas for straight line fitting, $y = a + bx$, are $a = \frac{S_{xx}S_y - S_x S_{xy}}{\Delta}$, $b = \frac{SS_{xy} - S_x S_y}{\Delta}$, $\Delta = SS_{xx} - (S_x)^2$, $\sigma_a^2 = \frac{S_{xx}}{\Delta}$, $\sigma_b^2 = S/\Delta$, where $S = \sum 1/\sigma_i^2$, $S_x = \sum \frac{x_i}{\sigma_i^2}$, etc.

   We transform the problem into standard linear fit form. First, if the error in f is σ_i the error is lnf is σ_i/f, so we need to change all σ_i is the standard formulas to σ_i/y_i. The rest is easy, a -> ln A, b -> -k. For the error in k, the formula work as it is. But for error in A, we need to use the error propagation formula to obtain A times the standard formula $\sqrt{S_{xx}/\Delta}$.

5. A harmonic oscillator subject to a random noise has the equations of motion for the position x and momentum p given by

   $\frac{dx}{dt} = \frac{p}{m}$,

   $\frac{dp}{dt} = -m\omega^2 x - \gamma p + \xi(t)$.

Here m is particle mass, ω is oscillator angular frequency, γ is damping coefficient, and $\xi(t)$ is random noise satisfying zero mean value and some variance to be determined.

a. If there is no noise, $\xi(t)$=0, give the forward Euler's integration method to solve the equation numerically. Specify the local truncation error.
b. If the noise is nonzero and is implemented as independent Gaussian random number at each time step, determine the variance of the random number such that equipartition theorem, $\langle\frac{p^2}{2m}\rangle = \frac{k_B T}{2}$ and $\langle\frac{m\omega^2 x^2}{2}\rangle = \frac{k_B T}{2}$, are recovered. Hint: in steady state, the energy of the oscillator, $\frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$, is a constant on average.

a) Euler method $x_{n+1} = x_n + p_n h/m + O(h^2)$; $p_{n+1} = p_n + (-m\omega^2 x_n - \gamma p_n)h + O(h^2)$, which map the point (x_n, p_n) to (x_{n+1}, p_{n+1}) with an error of order h^2, i.e., the local truncation error is of order h^2. b) We assume $p_{n+1} = p_n + (-m\omega^2 x_n - \gamma p_n)h + \xi_n + O(h^2)$, where the variance of the gaussian random noise is to be determined. Let's compute the difference of kinetic + potential energy between two steps, $E_{n+1} - E_n$ to the order of accuracy, i.e., to order h only as the method already has error of $O(h^2)$, we get $E_{n+1} - E_n = -\gamma\, p_n^2 h/m + \xi_n^2/(2m) + O(h^2)$. This quantity should be zero on average. Taken the average over the noise, we get $\langle\xi^2\rangle = 2\gamma \langle p^2\rangle h = 2m\gamma k_B T h$.

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