NATIONAL UNIVERSITY OF SINGAPORE

PC5215 – NUMERICAL RECIPES WITH APPLICATIONS

(Semester I: AY 2020-21)

Via Zoom on Monday 23 Nov 1:00-3:00pm Time Allowed: 2 Hours

INSTRUCTIONS TO STUDENTS

1. This assessment paper contains THREE questions and comprises THREE printed pages (including this cover page).
2. Students are required to answer ALL questions; each sub-question carry 10 marks.
3. Students should write the answers for each question on a new page. Scan or soft copies should be uploaded to LumiNUS.
4. This is an OPEN BOOK examination.
5. Calculators or software packages are allowed to use.

1. Consider a general multi-variable Gaussian probability distribution of the form

$$P(x) \propto \exp\left(-\frac{1}{2}x^T A x\right),$$

where x is a real column vector of dimension N, and A is real symmetric N by N matrix, the superscript T stands for matrix transpose. For definiteness, we consider the 3 by 3 matrix

$$A = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}$$

below for numerical computations.

   a. Show that the covariant matrix of the random vector x is given by the inverse of A, that is $C = \langle xx^T \rangle = A^{-1}$. Determine the inverse matrix A^{-1} for the 3 by 3 case given.
   b. Show that the covariant matrix C in general is positive semi-definite, i.e., $y^T C y \geq 0$ for all real vectors y.
   c. We can write the covariant matrix by Cholesky decomposition of the form $C = LL^T$, where L is a lower triangular matrix. Give a general algorithm to determine L from C. Find for the specific case of 3 by 3 matrix L.
   d. A sequence of uniformly distributed random numbers $\xi_1, \xi_2, \xi_3, \cdots$, from [0,1) are given, determine a transform using the random numbers through the help of matrix L, such that the resulting random vector x is given by the Gaussian distribution $\propto \exp\left(-\frac{1}{2}x^T A x\right)$ [Recall the Box-Muller method].

   a. *Several approaches are possible. The simplest is to make a change of variable by z = B^{-1} x, with B B^T = A^{-1} = C. This is possible because A is positive definite. After the variable transform, the distribution is an independent gaussian, for each component of z. And the Jacobian of the transform is a constant which does not influence the distribution after normalization. Alternatively, one can write Ax exp(-x^T A x) as the derivative of exp(-1/2 x^T A x) and then use integration by parts to calculate the covariant matrix <xx^T>. Lastly, one can introduce a generating function for the moments, by considering integral Z(b) = int dx exp(-1/2 x^T A x + b^T x), the integration can be done by a shift of x. The second derivative of b is the correlation. The inverse is (by hand or using Mathematica)* $C = A^{-1} = \begin{bmatrix} 3/4 & 1/2 & 1/4 \\ 1/2 & 1 & 1/2 \\ 1/4 & 1/2 & 3/4 \end{bmatrix}$.
   b. *y^T C y = y^T <x x^T> y = < (x^T y)^2 > ≥ 0. This is a square of something, clearly cannot be negative. This is fairly general and does not need the specific form of A or C.*

c. *Cholesky algorithm is given by Numerical Recipes in C, 2nd second, page 96.*

$$L = \begin{bmatrix} \sqrt{2} & 0 & 0 \\ -\frac{1}{\sqrt{2}} & \sqrt{3/2} & 0 \\ 0 & -\sqrt{2/3} & 2/\sqrt{3} \end{bmatrix}.$$

d. *Using L, we do transform as in part a (with LL^T=C=A^{-1}), by x = L z, here z is independent gaussian which can be generated using Box-Muller method. Then x will be multi-variable Gaussian distributed. Some students used eigenvalue decomposition instead of Cholesky decomposition. But I think Cholesky decomposition is better and faster.*

2. Consider the conjugate gradient (CG) method to determine iteratively the solution of a linear equation $Ax = b$, where A is a symmetric positive-definite real matrix.
   a. State the CG algorithm.
   b. Let matrix $A = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}$ and the column vector $b = \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix}$. Starting from the origin, $x_0 = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$, determine the solution x by CG iteration method. Give the sequence $x_0, x_1, x_2, \ldots$ and the steps leading to it.
   c. Verify that the two search direction vectors n_0 and n_1 obtained in part b following the algorithm in part a satisfy the conjugate condition, that is, $n_0^T A n_1 = 0$.

   This question is fairly routine, and everyone did it correctly. The algorithm is given in the lecture week 9 slides or in the paper by J. R. Shewchuk. This table shows the values of intermediate steps (use Shewchuk's notations):

step	*d*	*r*	*alpha*	*beta*	*x*
0	*(1,2,1)*	*(1,2,1)*	*3/2*		*(0,0,0)*
1	*(3.2,0,3/2)*	*(1,-1,1)*	*1/3*	*1/2*	*(3/2,3,3/2)*
2		*(0,0,0)*			*(2,3,2)*

3. In molecular dynamics, by following a rigorous Hamiltonian dynamics with a time-independent classical Hamiltonian $H(p, q)$, one can only simulate a micro-canonical ensemble with a fixed total energy.

a. Write down the Hamilton equations of motion of the system and show that the total energy $E = H(p, q) = K(p) + V(q)$ is a conserved quantity, i.e., the rate of change dE/dt is 0.

b. In order to simulate a canonical ensemble, various proposals have been made. One of them is the Nosé-Hoover dynamics, which is given by enlarging the phase space to have one extra degree ζ with the revised equations of motion,

$$\dot{q}_j = v_j = \frac{p_j}{m},$$
$$\dot{p}_j = F_j - \zeta p_j,$$
$$\dot{\zeta} = \frac{1}{\tau^2}\left(\frac{K}{K_0} - 1\right),$$

here j runs over the degrees of freedom, $K = \sum_j \frac{1}{2} m v_j^2$ is the total kinetic energy. Show that in this case, the conserved quantity is no longer the total energy but rather $F = H + K_0\left(\tau^2\zeta^2 + 2\int_0^t dt'\,\zeta(t')\right)$.

c. Based on the new conserved quantity proved in part b, given an argument that the distribution in phase space of (p, q) is canonical.

Not a very difficult question except part c.

a. The Hamilton equations of motion is $\dot{q}_j = \partial H/\partial p_j$, $\dot{p}_j = -\partial H/\partial q_j$. Thus, by chain rule of differentiation, $\frac{dE}{dt} = \frac{dH}{dt} = \sum_j \partial H/\partial q_j\, \dot{q}_j + \sum_j \partial H/\partial p_j\, \dot{p}_j$. Substituting the Hamilton equations of motion, we find that the two terms cancel, so the energy is a constant.

b. The process is nearly the same, except that dp/dt has an extra term due to the "friction". Thus, the energy is not a conserved quantity but equal to, $\frac{dH}{dt} = -2\zeta K$. This is cancelled by the derivative of the second $K_0\,(\ldots)$ term if we use the equation for ζ. So that the expression F is a new conserved quantity.

c. Since the energy is not conserved, it is not a micro-canonical ensemble. Some students get confused with the term "canonical transform" and differential 2-form. In fact, it has nothing to do with it. Since F is conserved, it is a "microcanonical distribution" is the quantity F. However, F have p, q, and ζ. If we eliminate ζ and considering the marginal distribution of (p,q) it will be a different distribution. Since dH/dt is not zero, it means the energy is not fixed and fluctuating. So it can be distributed canonically according to exp(-E/(k_B T)), but proof of it is non-trivial. I will just refer to the original papers of Nose and Hoover.

-- End -- (WJS)