NATIONAL UNIVERSITY OF SINGAPORE

PC5215 – NUMERICAL RECIPES WITH APPLICATIONS

(Semester I: AY 2023-24)

Time Allowed: 2 Hours

INSTRUCTIONS TO STUDENTS

1. Write your student number on the answer book. Do not write your name.
2. This assessment paper contains FIVE questions and comprises THREE printed pages (including this cover page).
3. Students must answer ALL questions; each question carries equal marks.
4. Students should write the answers for each question on a new page.
5. This is a CLOSED BOOK examination.
6. Non-programable calculators are allowed.

1. Answer briefly the following questions:
    a. In the IEEE 754 floating-point representation, infinities are defined. Explain why this is useful and give the bit pattern for 32-bit single precision representing $+\infty$.
    b. What is the computational complexity of the LU decomposition for a square matrix of $N \times N$?
    c. In Python function definition and use, explain the difference for argument passing, when the argument (or parameter) is a single number vs. a list.
    d. What is the local truncation error in the 4th-order Runge-Kutta method for solving first-order differential equations?
    e. Explain the "Stochastic Gradient Descent" method in machine learning.

a) Infinities are useful for distinguishing with NaN (not-a-number) and for certain calculations such as 1.0/0.0 or numbers larger than any allowed representation. It has the bit pattern for positive infinity as 0 1111 1111 000….00. Note the fractional part is 0. b) N^3 , c) if it is a single value, it is passed as a copy, so that the original is unrelated or unchanged. If it is passed as a list, only a reference is passed; any change in the function to the list is also reflected in the calling routine. d) $O(h^5)$. e) We move the weight according to negative gradient, W -> W – η ∇ L, where L is the loss function, η is a small number, and ∇ means taking the gradient. Stochastic means we use only part of the data to compute L. Repeated application minimizes L.

2. The Gauss quadrature is useful when the integrand decays fast. Consider the following integral using a three-point formula,

$$\int_{-\infty}^{+\infty} e^{-x^2} f(x)dx \approx \sum_{i=1}^{3} w_i f(x_i) .$$

   The orthogonal polynomials with the weight e^{-x^2} are the Hermite polynomials, $P_0 = 1$, $P_1 = 2x$, $P_2 = 4x^2 - 2$, and $P_3 = 8x^3 - 12x$. [You may use the formula $\int_{-\infty}^{+\infty} x^n e^{-x^2} dx = \sqrt{\pi}$ for $n = 0$, $\sqrt{\pi}/2$ for $n = 2$, or in general $\Gamma\left(\frac{1+n}{2}\right)$ for even n.]
    a. Determine the abscissas x_i and weights w_i.
    b. What polynomials can be integrated exactly? Give an order of magnitude estimate of the error of the formula.

a) abscissas are the roots of P_3, giving $x_1=0$, $x_{2,3} = \pm\sqrt{3/2}$. The weights are determined by using 1, x, x^2 to the formula, giving $w_1 + w_2 + w_3 = \sqrt{\pi}$, $w_1*0 + w_2(-\sqrt{3/2}) + w_3\sqrt{3/2}=0$, and $w_1*0+w_2*(3/2) + w_3*3/2 = \sqrt{\pi}/2$. Solve the equations, we find $w_1 = (2/3)\sqrt{\pi}$, $w_2=w_3 = \sqrt{\pi}/6$. b) The formula is exact for all polynomials up to order 5. Error occurs at x^6. Since there is no small parameter such as h in this problem, it is hard to quantify the error. We can use $\int_{-\infty}^{+\infty} e^{x^2} P_6 dx$ as a gauge.

3. A certain free-falling mechanics experiment found that the data can be fitted by $y = vt + \frac{1}{2}gt^2$, where y is height and t is time. The table below shows the experimental results. Use the data to determine the fitting parameters v and g.

Time t (sec)	Height y (m)
0.1	0.03705
1.1	5.9344
2.1	21.588
3.1	47.482

With the four different times, we get four linear equations for v and g of the form

$$\begin{pmatrix} 0.1 & 0.1^2/2 \\ 1.1 & 1.1^2/2 \\ 2.1 & 2.1^2/2 \\ 3.1 & 3.1^2/2 \end{pmatrix} \begin{pmatrix} v \\ g \end{pmatrix} = \begin{pmatrix} 0.03705 \\ 5.9344 \\ 21.588 \\ 47.482 \end{pmatrix}.$$

This is of the form of matrix equation Aa = b. We use the normal equation, $A^TAa = A^T b$, or $a = (A^TA)^{-1}(A^Tb)$. The numerical solution is v = - 0.16285, g = 9.9813. One can also minimizing the χ square, the result is the same.

4. We can compute numerically the derivative of a function by the central difference formula,

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}.$$

   a. What is the error of the formula due to a finite h, as a power of h?
   b. The definition of the derivative is that you take the limit $h \to 0$, but this cannot be performed on a computer. What is the optimal choice of h if the machine epsilon for the floating-point representation is ϵ?

a) Taylor expanding the right-hand side with h, we find (f(x+h) – f(x-h))/(2h) = f' + $f'''h^2/6$ + … So the error is $O(h^2)$. b) When the third order Tayler expansion due to a finite h are smaller than f times machine epsilon, we loss accuracy. f set the scale. The calculation must be accurate to order h^2. So the optimal choice for h is when $f'''h^3 \sim f\epsilon$, or when $h \approx \left(\frac{f\epsilon}{f'''}\right)^{1/3}$. See "Numerical Recipes in C", 2nd ed, Chap 5.7.

5. Consider a simple harmonic oscillator with the Hamiltonian $H = \frac{p^2}{2m} + \frac{1}{2}kx^2$.
   a. Based on the Hamilton's equations of motion and the Euler method for solving differential equations, present a first-order symplectic method.
   b. If, in addition to the usual spring restoration force $-kx$, there is a stochastic random force $\xi(t)$ of Langevin type, with $\langle \xi(t) \rangle = 0$, and $\langle \xi(t)\xi(t') \rangle = \frac{2\gamma k_B T}{m}\delta(t-t')$, where γ is the damping parameter, k_B is the Boltzmann constant, and T is temperature, how do the equations need to be modified? How can the Langevin equation be solved numerically on a computer?

a) The equation of motion is dp/dt = - kx, dx/dt = p/m. A symplectic method is $p_{n+1}=p_n-hkx_n$, $x_{n+1}=x_n+hp_{n+1}/m$. *b) The equation for p needs to be modified to be dp/dt =* $-kx - \gamma\frac{dx}{dt} + \xi(t)$. *Whenever a random force is added, we also need to add the damping force according to Stokes' law, so that the fluctuation-dissipation theorem is satisfied. We can use the Euler method as* $p_{n+1}=p_n-hkx_n - \gamma h p_n/m + B$. *The coordinate x is as in part a). Here B =* $\int_0^h \xi(t)dt$ *is a gaussian random number with zero mean and variance* $\langle B^2 \rangle = 2\gamma k_B T h/m$. *See week 13 slides, page 7.*

---The end --- [WJS]