PC5215 Numerical Recipes with Applications - Review Problems

1. Give the IEEE 754 single precision bit pattern (binary or hex format) of the following numbers:

   1.0 2.0 0.25 10.0 0.1 –0.01

   Note that it has 8 bits for the exponent, 24 bits precision (mantissa) with the leading one omitted in the representation, and a sign bit. The exponent is biased by 127.

   [Read the article "What Every Computer Scientist Should Know about Floating-Point Arithmetic".

   Ans:

   ```
   3F800000
   40000000
   3E800000
   41200000
   3DCCCCCD
   BC23D70A
   ```

   ]

2. Solve the following finite difference equation

   $$a x_{n+1} + b x_n + c x_{n-1} = 0 .$$

   The solution depends on two initial values, say, x_0 and x_1. Discuss the advantage and disadvantage of using the final solution to compute x_n versus recursion.

   [Hint: assuming $x_n = \mathrm{const}\, \lambda^{n}$.]

3. How to make a dynamic memory allocation for 2D array in C, say `a[n][m]`? What is machine ε? Run program `machar()` on page 892 to determine machine epsilon for your machine, what is roughly ε for single precision, double precision, or quadruple precision?

4. Do LU decomposition (without pivoting) of the following matrix by Crout's algorithm:

   $$\begin{bmatrix} 1 & 2 & -1 \\ 0 & 2 & 1 \\ 1 & -3 & 5 \end{bmatrix}.$$

   [Ans:

   $$L = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & -5/2 & 1 \end{bmatrix}, \quad U = \begin{bmatrix} 1 & 2 & -1 \\ 0 & 2 & 1 \\ 0 & 0 & 17/2 \end{bmatrix}$$

   ]

5. Give the computational complexity O(N^{k}) of the following algorithms (also state what is N), LU, Det(A) (by LU), A^{-1} (by LU) $Ax=b$ by Gaussian elimination, Neville's interpolation, Trapezoidal rule, FFT, conjugate gradient for linear system, quick sort, heap sort.

[Ans: N^3, N^3, N^3, N^3, N^2, N, $N \log N$, N^3, $N \log N$, $N \log N$]

6. What is the inverse of the following matrix?

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & a & 1 & 0 \\ 0 & b & 0 & 1 \end{bmatrix}.$$

[Use LU decomposition or otherwise directly by $AA^{-1} = I$. Ans.

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -a & 1 & 0 \\ 0 & -b & 0 & 1 \end{bmatrix}$$

]

7. Classify each of the following matrices as well-conditioned or ill-conditioned. Note that the condition number of a matrix is defined as $\|A\| \cdot \|A^{-1}\|$.

(a) $\begin{bmatrix} 10^{10} & 0 \\ 0 & 10^{-10} \end{bmatrix}$ (b) $\begin{bmatrix} 10^{10} & 0 \\ 0 & 10^{10} \end{bmatrix}$

(c) $\begin{bmatrix} 10^{-10} & 0 \\ 0 & 10^{-10} \end{bmatrix}$ (d) $\begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix}$

[Ans: the 2-norm condition numbers are, respectively, 10^{20}, 1, 1, ∞. Large condition number means ill-conditioning.]

8. What are the conditions required to the polynomials for cubic splines?
[Ans: function and its first derivative are continuous at the meeting points of each segment.]

9. Apply Neville's algorithm to determine the value $f(x)$ at x=1. The interpolation points are (0,1), (2,3), (3, 5). Determine also the polynomial (using Lagrange formula) in expanded form.
[Ans: $f(1) = 5/3$, $f(x) = 1 + x/3 + x^2/3$.]

10. Prove the open formula:

$$\int_{x_0}^{x_1} f(x)dx = h f_1 + O(h^2),$$

$$\int_{x_0}^{x_1} f(x)dx = h\left[\frac{3}{2} f_1 - \frac{1}{2} f_2\right] + O(h^3),$$

[Hint: use Taylor expansion.]

11. What is the basic idea of Guassian integration? Derive a 2-point formula for the Guassian integral in the interval [–1,1] with a constant weight $W(x)$=1.
[Ans: $x_1 = -x_2 = 1/\sqrt{3}, \quad w_1 = w_2 = 1$.]

12. Write out the steps for quick sort and heap sort, for the following input data:
[1, 5, 3, 6, 7, 2, 9, 0, 4, 8].

13. What is the computational complexity of the Newton-Raphson method for the root **x** (such that **F**(**x**) =**0**) in N dimensions? Derive the formula for the iteration. Discuss issue on stability.
[Ans: N^3. $\mathbf{x} \leftarrow \mathbf{x} - \mathbf{J}^{-1}\mathbf{F}, \quad \mathbf{J} = \partial \mathbf{F} / \partial \mathbf{x}$.]

14. Compute the solution of $x^2 - 2 = 0$ numerically using Newton's method, starting from x=1. Need a calculator for this.
[Ans: Iterate $x \leftarrow x/2 + 1/x$, after three iterations, one gets 1.41422.]

15. How to bracket a zero, bracket a minimum, or maximum?

16. Consider the function $f(x,y) = x + x^2 - xy + y^2$. Use the conjugate gradient method to find the minimum of the above function, starting from the point (x_0,y_0)=(1,1).

17. Show that the error at i-th step in the conjugate gradient method is of the form
$e_{(i)} = \sum_{j=i}^{N-1} \delta_j d_{(j)}$, where $d_{(j)}$ is the search direction in the j-th step.
[Read the article by J. R. Shewchuk, "An introduction to the conjugate gradient method without the agonizing pain."]

18. Prove that the optimal condition to stop in a linear search (in higher dimensions) is that $\mathbf{n} \cdot \mathbf{g} = 0$, where **n** is search direction, **g** is the gradient at the new location.
[Hint: derivative with respect to λ of $f(\mathbf{x}+\lambda\mathbf{n})$ is zero at min or max.]

19. (a) Solve the system of equations (in least squares sense):

$$x + y = 3$$
$$2x + 3y = 5$$
$$3x - y = 2$$

(b) Solve the same problem by conjugate gradient method (as a minimization problem).
[Ans: x=1.0507, y=1.0725.]

20. Do the FFT steps for the following input:
[1, –2, –1, 1, –1, –2, 2, 1].

21. A set of data points is given as following:
(0, 0.01), (1, 1.02), (2, 1.98), (3, 3.10), (4, 4.22)

Determine a straight line (least-squares) fit $f(x) = a+bx$, give also the error estimates of the fitting parameters a and b. Is there any relation between the current problem and Prob 19?
[Ans: $a = 1.05 \pm 0.02, b = -0.034 \pm 0.050$.]

22. Consider discretized version of the equation dy/dx= $-y$ using forward difference and backward difference:

$$y_{n+1} = y_n - h y_n$$
$$y_n = y_{n-1} - h y_n$$

Solve the difference equations exactly and compare them with exact solution of the differential equation. Which version is preferred?
[Ans: forward difference $y_n = (1-h)^n y_0$, backward difference $y_n = (1+h)^{-n} y_0$. Exact solution is $y(nh) = y_0\exp(-nh)$. The second backward difference method is preferred, due to its stability (errors do not blow up) for any step size h.]

23. Consider the Hamiltonian

$$H(p,q) = \frac{1}{2}\left(p^2 + q^2\right).$$

Give a second order symplectic algorithm for solving this system. Show that the resulting update viewed as a transformation in the phase space (p,q) preserves the phase space area. Show explicitly that it is symplectic ($D^T JD = J$ or $dp \wedge dq$ is invariant with respect to the transformation, where D is Jacobian matrix of the transformation and the matrix

$$J = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}).$$

[Ans: The Hamilton's equations of motion are $dp/dt = -\partial H/\partial q = -q$, $dq/dt = \partial H/\partial p = p$, so

$$q' = q + hp - h^2 q/2$$
$$p' = p - h(q+q')/2 .$$

We can show that the Jacobian of the above transformation from (p,q) to (p',q') is 1, so area is preserved. That is, we can verify that Det(D)=1:

$$\text{Det}(D) = \begin{vmatrix} \dfrac{\partial p'}{\partial p} & \dfrac{\partial p'}{\partial q} \\ \dfrac{\partial q'}{\partial p} & \dfrac{\partial q'}{\partial q} \end{vmatrix} = \begin{vmatrix} 1-\dfrac{h^2}{2} & -h+\dfrac{h^3}{4} \\ h & 1-\dfrac{h^2}{2} \end{vmatrix} = 1 .$$

And

$$dp' \wedge dq' = d[(1-h^2/2)p + (-h+h^3/4)q] \wedge d[(1-h^2/2)q + hp]$$
$$= (1-h^2/2)(1-h^2/2)\, dp \wedge dq + (-h+h^3/4)h\, dq \wedge dp$$
$$= dp \wedge dq$$

(Since $dp \wedge dp = 0, dq \wedge dq = 0, dp \wedge dq = -dq \wedge dp$.)
]

24. Generate points distributed uniformly on a unit sphere ($x^2+y^2+z^2=1$).

25. Given that ξ_1 and ξ_2 are independent, uniformly distributed random variables between 0 and 1, what are the probability distributions of the random variables $\xi_1 + \xi_2$ and $\xi_1 \times \xi_2$?
[Ans: for $\xi_1 + \xi_2$ case, consider $P(\xi_1 + \xi_2 < x) = F(x)$, $p(x) = dF(x)/dx = x$ for $0 < x < 1$, $2-x$ for $2 > x > 1$.]

26. Write down the transition matrix W for a one-dimensional 4-spin Ising model with periodic boundary condition using Metropolis flip rate.

27. (a) Let assume W_i has invariant distribution P for all i, i.e., $P = P\,W_i$, $i=1,2,..,N$. Show that both $W_s = \Sigma\lambda_i W_i$ and $W_p=\Pi W_i$ has invariant distribution P, where $\Sigma\lambda_i=1$ and $\lambda_i>0$. How to implement W_s and W_p on computer? (b) If W_i satisfies detailed balance with respect to P, does W_s and/or W_p satisfy detailed balance?