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, 23 bits of factional part (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. IEEE floating-point number of half precision contains 16 bits, with the highest bit for the sign, 5 bits for the biased exponent, and the remaining 10 bits for the fractional part. Based on this information, determine the following:

   a. the machine epsilon,
   b. the largest possible value,
   c. work out the bit pattern for the numerical value of $\pi \approx 3.141592653$. How many digits are exactly represented with half precision for π?

   a) $\epsilon = 2^{-10} \approx 10^{-3}$ *b) 0 11110 1111111111 in bits which is* $2^{15}(2 - 2^{-10}) = 2^{16} - 32 = 65504$. *c) sign = 0, biased exponent e = 15 + 1 = 16, 3 -> 11, 0.14159… = 0.001001000011, so the IEEE bit pattern is 0 10000 1001001000 which is 3.140625 accurate to 3 digits.*

3. The IEEE 754 single-precision floating point has a sign bit, followed by 8 bit for the biased exponent, and 23 bits for the fractional part. What is the decimal value for the following bit pattern:
   100 1 0010 0000 0000 0000 0000 0000 = ?

4. We consider the IEEE floating point arithmetic on computer.
   a. In single precision, the highest bit represents a sign, the next 8 bits give the biased exponent, and the remaining 23 bits are the fractional part. Work out the presentations for the decimal numbers $x = 0.1$, $y = 0.25$, and $z = 0.3$.
   b. Floating point addition does not obey associativity. As a result, in general, $(x + y) + z \neq x + (y + z)$. Assuming exact rounding for addition on computer, compute the difference $\Delta = [(x + y) + z] - [x + (y + z)]$.

5. 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 $x_n = \text{const}\ \lambda^n$.]

6. 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:

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

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7. Give the computational complexity, i.e., the power in 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, $N \log N$, $N \log N$]

8. 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.

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

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9. 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.]

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

11. 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: $f(1) = 5/3$, $f(x) = 1 + x/3 + x^2/3$.]

12. (a) Consider interpolating 4 points (x,y) = (0,1), (1,1), (2,1), (3,1) with a polynomial of degree 3 or less, without actually going through any calculation, what should be that polynomial?
    (b) Based on the observation of the result in (a), show that $\sum_{i=1}^{N} l_i(x) = 1$ for any x and N, where $l_i(x)$ is the Lagrange interpolation polynomials in the Lagrange's formula $f(x) = \sum_{i=1}^{N} l_i(x) y_i$. You don't need the specific form of $l_i(x)$ to prove this.

13. 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.]

14. What is the accuracy of the rectangular integration rule (equally spaced abscissas):

$$\int_{x_0}^{x_N} f(x)dx = \frac{(x_N - x_0)}{N} \sum_{i=0}^{N-1} f_i + O\left(\frac{1}{N^?}\right)?$$

    I.e., find the power k in the error term $O(1/N^k)$. Steps and justifications are required.

15. 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: $x_1 = -x_2 = 1/\sqrt{3}, \quad w_1 = w_2 = 1$.]

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

17. 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.]

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

19. 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 $(x_0,y_0)=(1,1)$.

20. 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."]

21. 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 the 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.]

22. (a) Solve the system of equations (in the least squares sense):
$$x + y = 3$$
$$2x + 3y = 5$$
$$3x - y = 2$$
(b) Solve the same problem by the conjugate gradient method (as a minimization problem).
[Ans: $x=1.0507$, $y=1.0725$.]

23. 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 22?
[Ans: $a = 1.05 \pm 0.02, b = -0.034 \pm 0.050$.]

24. Consider the discretized version of the equation dy/dx= –y using forward difference and backward difference:

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

Solve the difference equations exactly and compare them with the 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.]

25. 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

$$\begin{aligned} q' &= q + hp - h^2 q/2 \\ p' &= p - h(q+q')/2 \end{aligned}.$$

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:

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

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 $dp \wedge dp = 0,\ dq \wedge dq = 0,\ dp \wedge dq = -dq \wedge dp$.)

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

27. 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 $2 > x > 1$.]

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

29. (a) Let us 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?

30. Consider a Markov chain given by the transition matrix

$$W = \begin{bmatrix} 1/2 & 1/4 & 0 & 1/4 \\ 0 & 1/3 & 2/3 & 0 \\ 0 & 1 & 0 & 0 \\ 1/2 & 0 & 1/2 & 0 \end{bmatrix}.$$

   a. Is the Markov chain irreducible?
   b. Does the Markov chain have an invariant or equilibrium distribution? If so, determine the invariant distribution.

31. Consider the concepts in Markov chain Monte Carlo.
   a. Define irreducibility, and define aperiodicity.
   b. Is the Markov chain specified by the transition matrix W below irreducible? aperiodic?

$$W = \begin{bmatrix} 1/2 & 1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 1/3 & 2/3 \\ 0 & 0 & 1/3 & 2/3 \end{bmatrix}$$

   c. Determine invariant states p such that $pW = p$. Here p is a row vector defines the probabilities of the four states.