

# Mathematics for Chemistry: Exam Set 1

March 19, 2017

## 1 mark Questions

- The maximum value of the rank of any  $5 \times 3$  matrix is  
(a) 2 (b) 3 (c) 4 (d) 5
- The determinant of an identity  $n \times n$  matrix is equal to  
(a) 1 (b) -1 (c) 0 (d) n
- A square matrix  $M$  that satisfies  $M^T = M^{-1}$  is a  
(a) symmetric matrix (b) orthogonal matrix (c) skew-symmetric matrix (d) Hermitian matrix
- The kind of errors that can be quantified using error estimates are  
(a) gross errors only (b) random errors only (c) systematic errors only (d) systematic and random errors
- The standard error of mean in terms of the standard deviation  $\sigma$  for  $N$  measurements is equal to  
(a)  $\sigma/N$  (b)  $\sigma/(N-1)$  (c)  $\sigma/\sqrt{N}$  (d)  $\sigma/\sqrt{N-1}$
- Which of the following is NOT the characteristic of a conservative force  
(a) Work done by force in performing a displacement is independent of path.  
(b) Force can be expressed as the gradient of a potential.  
(c) Force between two particles satisfies law of equal action and reaction.  
(d) Net force on a particle is constant during the motion.
- The correct relation between a surface integral over a surface  $S$  and the line integral over a closed region  $C$  enclosing a surface  $S$  is given by  
(a)  $\oint_C \vec{f} \cdot d\vec{r} = \iint_S \vec{f} \cdot \hat{n} \, dx dy$   
(b)  $\oint_C \vec{\nabla} \times \vec{f} \cdot d\vec{r} = \iint_S \vec{f} \cdot \hat{n} \, dx dy$   
(c)  $\oint_C \vec{\nabla} \times \vec{f} \cdot d\vec{r} = \iint_S \vec{\nabla} \times \vec{f} \cdot \hat{n} \, dx dy$   
(d)  $\oint_C \vec{f} \cdot d\vec{r} = \iint_S \vec{\nabla} \times \vec{f} \cdot \hat{n} \, dx dy$
- According to potential theory, a differential  $dW = A dx + B dy$  is exact if  
(a)  $\frac{\partial A}{\partial y} = \frac{\partial B}{\partial x}$   
(b)  $\frac{\partial A}{\partial y} = -\frac{\partial B}{\partial x}$   
(c)  $\frac{\partial A}{\partial x} = \frac{\partial B}{\partial y}$   
(d)  $\frac{\partial A}{\partial x} = -\frac{\partial B}{\partial y}$
- The statement below that is NOT an axiom for a real vector space is  
(a) Addition of two vectors yields another vector  
(b) Scalar (real number) multiplication of a vector yields another vector  
(c) Addition of vectors is commutative  
(d) Product of two vectors yields a scalar (real number)

10. The correct statement below regarding divergence is correct is  
 (a) Divergence of a scalar field produces a vector field.  
 (b) Divergence of a vector field produces a scalar field.  
 (c) Divergence of a vector field produces a vector field.  
 (d) Divergence of a scalar field produces a scalar field.
11. The number of arbitrary constants in the particular solution of a 2nd order ordinary differential equation is  
 (a) 0 (b) 1 (c) 2 (d)  $\infty$
12. The equation  $x dx + (x^2 + 1)dy = 0$  is an example of a (ODE stands for Ordinary Differential Equation)  
 (a) nonlinear homogeneous 1st order ODE  
 (b) nonlinear nonhomogeneous 1st order ODE  
 (c) linear homogeneous 1st order ODE  
 (d) linear nonhomogeneous 1st order ODE
13. The correct statement below regarding 1st order ODEs is  
 (a) Any 1st order ODE can be written in terms of an exact differential by variation of parameters.  
 (b) It is possible to express any 1st order homogeneous ODE in the separable form  $A(y)dy = B(x)dx$ .  
 (c) Any 1st order ODE can be solved by variation of parameters.  
 (d) Given any 1st order ODE it is possible to find an integrating factor that depends only on  $x$ .
14. The 2nd order differential equation below that can be solved using a trial solution of the form  $y = x^m$  is  
 (a)  $y'' + 2xy' + 2y = 0$   
 (b)  $y'' + 2y' + 2y = 0$   
 (c)  $y'' + (2/x)y' + (2/x^2)y = 0$   
 (d)  $y'' + (2/x^2)y' + (2/x)y = 0$
15. The trial solution for the differential equation  $y'' - 3y' + 2y = 0$  is of the form ( $\lambda$  is a parameter)  
 (a)  $\lambda x$  (b)  $x^\lambda$  (c)  $e^{\lambda x}$  (d)  $\lambda - (2\lambda x/3)$
16. Consider the differential equation  $y'' + 4y = 0$ . If the two linearly independent solutions are expressed as real functions  $\sin(2x)$  and  $\cos(2x)$ , the absolute value of the Wronskian is equal to  
 (a)  $|\sin(2x)|$  (b) 2 (c)  $|2\sin(x)|$  (d) 1
17. The power series method is typically used to obtain  
 (a) a second linearly independent solution of a 2nd order ODE when the first solution is known  
 (b) the solution of a nonhomogeneous second order ODE when the solution of the corresponding homogeneous ODE is known  
 (c) the general solution of a homogeneous second order ODE  
 (d) the general solution of a homogeneous second order ODE with constant coefficients
18. The Frobenius method can be applied about the point  $x = 0$  for the differential equation  
 (a)  $y'' + y'/x^2 + y/x^2 = 0$   
 (b)  $y'' + y'/x + y/x^3 = 0$   
 (c)  $y'' + y'/x + y/x^2 = 0$   
 (d)  $y'' + y'/x^2 + y/x = 0$
19. The orthogonality condition for Legendre polynomials  $P_n(x)$  and  $P_m(x)$  when  $m \neq n$  is  
 (a)  $\int_{-\infty}^{+\infty} x^2 P_n(x) P_m(x) dx = 0$

- (b)  $\int_{-1}^{+1} P_n(x)P_m(x)dx = 0$   
 (c)  $\int_{-1}^{+1} (1 - x^2)P_n(x)P_m(x)dx = 0$   
 (d)  $\int_{-\infty}^{+\infty} P_n(x)P_m(x)dx = 0$

20. The equation  $x^2y'' + xy' + x^2y = 0$  is an example of  
 (a) Legendre equation (b) Bessel equation (c) Hermite equation (d) Leguerre equation

## 2 mark Questions

1. An experiment is repeated several times and the readings are recorded. The readings are 5.01, 4.95, 4.99, 5.03, 5.02. Based on this data, we infer that the type of error in the measurement is most likely to be a  
 (a) Systematic Error (b) Random Error (c) Gross Error (d) Cannot infer the type of error

2. A quantum mechanical particle in a 2D box has the following probability distribution

$$p(x) = A \sin^2(2\pi x) \sin^2(2\pi y) \quad \text{for } 0 \leq x \leq 2 \text{ and } 0 \leq y \leq 2$$

$$= 0 \quad \text{otherwise}$$

where  $A$  is some constant and the value of  $\pi$  can be taken as 3.14. The value of  $A$  so that the distribution is normalized is

- (a) 1 (b) 2 (c) 1/2 (d) 1/4
3. The average speed of a certain gas at some temperature is 100 m/s. The gas molecules follow a Maxwell-Boltzmann distribution of speeds we can assume  $\pi = 3.14$ . The probability distribution of speeds  $u$  (expressed in m/s) is proportional to  
 (a)  $e^{-u^2/15700}$  (b)  $u^2e^{-u^2/15700}$  (c)  $e^{-u^2/31400}$  (d)  $u^2e^{-u^2/31400}$
4. A real inner product of two arbitrary vectors  $a$  and  $b$  is denoted by  $(a, b)$ . We present three conditions below  
 (A)  $(a, a) \geq 0$  for all  $a$   
 (B)  $(a, b) = (b, a)$  for all  $a$  and  $b$   
 (C)  $(a, b)^2 \leq (a, a)(b, b)$   
 The conditions that need to be satisfied for  $(a, b)$  to be a valid definition of the inner product are  
 (a) A, B and C  
 (b) B and C, but not A  
 (c) A and C, but not B  
 (d) A and B, but not C
5. The force on a particle at the point (1,1,1) due to the potential

$$V(x, y, z) = \frac{1}{2}(x^2 + y^2 + z^2)$$

is equal to

- (a)  $(1/9)(\hat{i} + \hat{j} + \hat{k})$   
 (b)  $(1/4)(\hat{i} + \hat{j} + \hat{k})$

(c)  $(-1/9)(\hat{i} + \hat{j} + \hat{k})$

(d)  $(-1/4)(\hat{i} + \hat{j} + \hat{k})$

6. Consider a vector field given by  $\vec{v} = yz\hat{i} + xz\hat{j} + xy\hat{i}$ . The divergence of this field at the point (1,1,1) is equal to

(a) 3 (b) 1 (c) -3 (d) 0

7. Consider the three forces below:

(A)  $2x^2\hat{i} + (4xy + y^2)\hat{j}$

(B)  $(4xy + x^2)\hat{i} + 2x^2\hat{j}$

(C)  $3(x^2/y)\hat{i} - (x^3/y^2)\hat{j}$

The forces which are conservative are

(a) A,B and C

(b) B and C but not A

(c) B only

(d) C only

8. According to the first two laws of thermodynamics, we have the change in enthalpy  $dH$  related to the change in pressure  $dP$  and the change in entropy  $dS$  via  $dH(P, S) = V(P, S)dP + T(P, S)dS$ . The condition for  $H(P, S)$  to be an exact differential gives the relation

(a)

$$\frac{\partial V}{\partial P} = \frac{\partial S}{\partial T}$$

(b)

$$\frac{\partial V}{\partial S} = \frac{\partial T}{\partial P}$$

(c)

$$\frac{\partial V}{\partial T} = \frac{\partial S}{\partial P}$$

(d)

$$\frac{\partial V}{\partial S} = \frac{\partial S}{\partial P}$$

9. The wave function of an electron in the Hydrogen atom in the  $2p_z$  orbital in spherical polar coordinates is proportional to  $\cos\theta(r/a_0)e^{-r/2a_0}$  where  $a_0$  is a constant. The volume integral of the *square* of this function over all space is equal to (use the result  $\int_0^\infty x^n e^{-x} dx = n!$ )

(a)  $32\pi a_0^3$  (b)  $4\sqrt{2\pi}a_0^{3/2}$  (c)  $\frac{1}{32\pi a_0^3}$  (d)  $\frac{1}{4\sqrt{2\pi}a_0^{3/2}}$

10. Consider the matrix

$$\begin{pmatrix} 1 & b & 0 & b \\ b & 1 & b & 0 \\ 0 & b & 1 & b \\ b & 0 & b & 1 \end{pmatrix}$$

where  $b$  is some real number. The above matrix is

(a) symmetric but not orthogonal

(b) orthogonal but not symmetric

(c) both symmetric and orthogonal

(d) neither symmetric nor orthogonal

11. Consider the following set of equations:

$$\begin{aligned}4x + 3y + z &= 4 \\x - 4y + 2z &= 10 \\3x + 7y - z &= -5\end{aligned}$$

The set of equations above has

- (a) no solution
- (b) a unique solution
- (c) multiple (but finite) number of solutions
- (d) infinite number of solutions

12. Consider a vector in 3D (1,0,1). When this vector is rotated by  $45^\circ$  about the Y-axis, the resulting vector is closest to (a) (0,0,1.41) (b) (1.41,0,0) (c) (1.41,0,1.41) (d) (1.41,1.41,1.41)

13. The eigenvalues of the matrix

$$\begin{pmatrix} 1 & 3 \\ 4 & 2 \end{pmatrix}$$

are

- (a) 2 and 1 (b) 2 and -1 (c) 5 and -2 (d) 5 and 2

14. The particular solution of the differential equation  $y'x = 2y - 4$  with the boundary condition  $y(1) = 5$  is

- (a)  $y = 3x + 1$  (b)  $y = 3x^2 - 2$  (c)  $y = x^2 + 4$  (d)  $y = 3x^2 + 2$

15. The integrating factor below that converts the differential  $(2xy + \sin x)dx + \cos y(\cos x \tan y + x^2 - x^2y \tan y)dy$  to an exact differential is

- (a)  $\sin x$  (b)  $\cos x$  (c)  $\sin y$  (d)  $\cos y$

16. The system of 1st order ODEs

$$\frac{dx}{dt} = xy + t$$

$$\frac{dy}{dt} = xt$$

can be written as the second order ODE

(a)

$$\frac{d^2y}{dt^2} = xt + xyt$$

(b)

$$\frac{d^2y}{dt^2} = xt + t^2$$

(c)

$$\frac{d^2y}{dt^2} = xt + xyt + t^2$$

(d)

$$\frac{d^2y}{dt^2} = x^2y^2 + txt$$

17. The system of DEs

$$\frac{dx}{dt} = x + 2y$$

$$\frac{dy}{dt} = 2x + y$$

has a general solution of the form (where  $A$  and  $B$  are arbitrary constants)

(a)

$$Ae^x + Be^{-3x}$$

(b)

$$Ae^{-x} + Be^{3x}$$

(c)

$$Ae^{ix} + Be^{-3ix}$$

(d)

$$Ae^{-ix} + Be^{3ix}$$

18. The second order ODE  $y'' + 4y = \sin x$  has a general solution of the form (where  $A$  and  $B$  are arbitrary constants)

(a)

$$A \sin 2x + B \cos 2x + \sin x$$

(b)

$$A \sin x + B \cos x - \sin x$$

(c)

$$A \sin 2x + B \cos 2x + \frac{1}{3} \sin x$$

(d)

$$A \sin 2x + B \cos 2x + 1$$

19. The indicial equation for the differential equation

$$x^2 y'' + xy' + x^2 y = 0$$

solved using the Frobenius method with a trial solution  $y = \sum_{i=0}^{\infty} c_n x^{n+r}$  is

(a)

$$r^2 - r = 0$$

(b)

$$r^2 - r - 1 = 0$$

(c)

$$r^2 - 1 = 0$$

(d)

$$r^2 = 0$$

20. Based on the Rodrigues formula

$$P_n(x) = \frac{(-1)^n}{2^n n!} \frac{d^n}{dx^n} (1-x^2)^n$$

, the form of  $P_3(x)$  is

(a)

$$\frac{1}{2} (5x^3 - 2x^2 + 3x)$$

- (b)  $\frac{1}{2}(x^3 - 3x)$
- (c)  $\frac{1}{2}(5x^3 - 3x)$
- (d)  $\frac{1}{2}(5x^5 + x^3 - 3x)$

## 4 mark questions

1. Solving the ODE

$$(1 - x^2)y'' - 2xy' + 2y = 0$$

for using the power series method with the trial solution

$$y = \sum_{n=0}^{\infty} a_n x^n$$

we get the recursion relation

- (a)  $a_{n+2} = \frac{(n+1)(n+2) - 2}{(n+1)(n+2)} a_n$
- (b)  $a_{n+2} = \frac{(n+1)n - 2}{(n+1)(n+2)} a_n$
- (c)  $a_{n+2} = \frac{(n+1)(n+2) - 6}{(n+2)(n+3)} a_n$
- (d)  $a_{n+2} = \frac{(n+1)n - 6}{(n+2)(n+3)} a_n$

2. If  $H_1(x)$  and  $H_2(x)$  are Hermite polynomials of order 1 and 2 respectively, the value of

$$\int_{-\infty}^{+\infty} H_1(x)xH_2(x)e^{-x^2} dx$$

is equal to

- (a) 0 (b) 1 (c)  $\sqrt{\pi}$  (d)  $4\sqrt{\pi}$

3. The correct statement regarding solution of the ODE

$$(1 - x^2)y'' - 2xy' + 2y = 0$$

using the Frobenius method ( $y = \sum_{n=0}^{\infty} a_n(x-1)^{n+r}$  about the point  $x = 1$  is

- (a) The equation can be solved using the Frobenius method with  $r = 0$  about the point  $x = 1$ .
- (b) The equation can be solved using the Frobenius method about the point  $x = 1$  but  $r \neq 0$ .
- (c) The equation cannot be solved using the Frobenius method about the point  $x = 1$ .
- (d) There is not enough information to decide whether the equation can be solved using the Frobenius method about the point  $x = 1$ .

4. The general solution of the second order nonhomogeneous equation

$$y'' + 16y = 4 \tan(4x)$$

is ( $A$  and  $B$  are arbitrary constants)

(a)

$$y = A \sin(4x) + B \cos(4x) + \sin(4x) \cos(4x)$$

(b)

$$y = A \sin(4x) + B \cos(4x) + \frac{\cos(4x)}{4} \ln\left(\frac{1 + \sin(4x)}{\cos(4x)}\right)$$

(c)

$$y = A \sin(4x) + B \cos(4x) + \frac{\sin(4x)}{4} \ln\left(\frac{1 + \sin(4x)}{\cos(4x)}\right)$$

(d)

$$y = A \sin(4x) + B \cos(4x) + \ln(\tan(4x))$$

5. The particular solution of the ODE

$$\frac{dy}{dx} = \frac{9x^2 - 2xy}{2y + x^2 + 1}$$

with boundary conditions  $y(0) = 0$  is

(a)

$$y^2 - yx^2 + 3x^3 = 0$$

(b)

$$y^2 + y(x^2 + 1) - 3x^2 = 0$$

(c)

$$y^2 - y(x^2 + 1) - x^3 = 0$$

(d)

$$y^2 + y(x^2 + 1) - 3x^3 = 0$$

6. Consider the matrix:

$$\begin{pmatrix} 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \end{pmatrix}$$

The inverse of this matrix is equal to

(a)

$$\begin{pmatrix} 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \end{pmatrix}$$

(b)

$$\begin{pmatrix} 1 & 1 & 0 & 1 \\ -1 & 1 & 1 & 0 \\ 0 & -1 & 1 & 1 \\ -1 & 0 & -1 & 1 \end{pmatrix}$$

(c)  $\frac{1}{3}$

$$\begin{pmatrix} 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \end{pmatrix}$$



(d)  $\frac{1}{3}$

$$\begin{pmatrix} 1 & 1 & 0 & 1 \\ -1 & 1 & 1 & 0 \\ 0 & -1 & 1 & 1 \\ -1 & 0 & -1 & 1 \end{pmatrix}$$

7. The probability density of finding a particle at the point  $(x, y, z)$  in a 3D rectangular box located between  $x = 0$  to  $x = 1$ ,  $y = 0$  to  $y = 2$  and  $z = 0$  to  $z = 1$  is equal to  $A \sin^2(\pi x) \sin^2(\pi y/2) \sin^2(\pi z)$  where  $A$  is a real number. The value of  $A$  so that this function is normalized is (a) 1 (b) 1/2 (c) 2 (d) 4
8. The differential work done  $dW$  in expanding a gas reversibly is given as  $-PdV$  where  $P$  is the pressure and  $dV$  represents the change in volume. The work done in expanding a gas from an initial pressure of  $10^5$  Pa and initial volume of 1 L to a final pressure of  $2 \times 10^5$  Pa and final volume of 0.5 L along a straight line path (in P-V space) is equal to (in J)  
(a) 100 (b) 75 (c) 300 (d) 200