Introduction to Mathematical Biophysics

Final Exam, Fall 2004

If a calculation is required, you can either use Maple or do the calculation by hand. In either case, explain the calculation that you did to get the answer.

Definitions:

Prime $'$ indicates matrix transpose.

Exact means the exact value, no decimals.

The rotation matrix in 2D is defined by

$$R(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

(1) Let

$$v_1 = (-1,-1,2)' \qquad v_2 = (1,1,3)' \qquad v_3 = (1,-2,-1)'$$

be consecutive points on a discrete curve. Find the matrix giving the discrete Frenet frame at v_2.

Solution:

$$\begin{bmatrix} 0 & -2/5\sqrt{5} & 1/5\sqrt{5} \\ -3/5 & -\frac{4}{25}\sqrt{5} & -\frac{8}{25}\sqrt{5} \\ -4/5 & \frac{3}{25}\sqrt{5} & \frac{6}{25}\sqrt{5} \end{bmatrix}$$

$$\begin{bmatrix} 0.0 & -0.8944271908 & 0.4472135954 \\ -0.6000000000 & -0.3577708763 & -0.7155417526 \\ -0.8000000000 & 0.2683281572 & 0.5366563145 \end{bmatrix}$$

(2) Let

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \qquad B = \begin{pmatrix} e & f \\ g & h \end{pmatrix}$$

a) Find the trace of AB

b) Find the trace of BA

Solution: $ae + bg + cf + dh$

(3) Find the exact value of the coefficients c_2 and c_{-2} for the Fourier series

$$\sum_{n=-\infty}^{\infty} c_n \exp(2\pi i n t)$$

of t^3 on the interval $0 \leq t \leq 1$.

Solution:

$$1/32\,\frac{8\,i\pi^2+6\,\pi-3\,i}{\pi^3}, -1/32\,\frac{8\,i\pi^2-6\,\pi-3\,i}{\pi^3}$$

(4) a) Let

$$a_k = \exp(-\pi i k).$$

and

$$N = 100.$$

Sketch below a graph of the function

$$f(x) = \sum_{-N}^{N} a_k \exp(2\pi i k x)$$

on the interval $0 \leq x \leq 1$. If f is interpreted as the one dimensional electron density in the interval $0 \leq x \leq 1$, at what coordinate is the atom located?

b) Let

$$g(x) = \sum_{-N}^{N} |a_k| \exp(2\pi i k x)$$

where a_k is as in part a). Sketch below a graph of $g(x)$ on the interval $0 \leq x \leq 1$. If g is interpreted as the one dimensional electron density in the interval $0 \leq x \leq 1$, at what coordinate is the atom located?

(5) Let

$$G = \begin{bmatrix} 2 & -1 & 3 \\ -1 & 2 & -1 \\ 3 & -1 & 2 \end{bmatrix}.$$

Find a matrix M such that

$$G = M'M.$$

Solution:

$$\begin{bmatrix} \frac{\sqrt{14+2\sqrt{17}}}{\sqrt{34-6\sqrt{17}}} & -1/2\,\frac{(-3+\sqrt{17})\sqrt{14+2\sqrt{17}}}{\sqrt{34-6\sqrt{17}}} & \frac{\sqrt{14+2\sqrt{17}}}{\sqrt{34-6\sqrt{17}}} \\ \frac{\sqrt{14-2\sqrt{17}}}{\sqrt{34+6\sqrt{17}}} & 1/2\,\frac{(3+\sqrt{17})\sqrt{14-2\sqrt{17}}}{\sqrt{34+6\sqrt{17}}} & \frac{\sqrt{14-2\sqrt{17}}}{\sqrt{34+6\sqrt{17}}} \\ -1/2\,i\sqrt{2} & 0 & 1/2\,i\sqrt{2} \end{bmatrix}$$

$$\begin{bmatrix} 1.549852967 & -0.8703242935 & 1.549852967 \\ 0.3129788827 & 1.114690820 & 0.3129788827 \\ -0.7071067810\,i & 0.0 & 0.7071067810\,i \end{bmatrix}$$

(6) Find a symmetric matrix to represent the quadratic function

$$6x^2 + 17y^2 + 5z^2 + 6xy - 16yz.$$

Find the principal values to 2 decimal places.

Solution:

$$G = \begin{bmatrix} 6 & 3 & 0 \\ 3 & 17 & -8 \\ 0 & -8 & 5 \end{bmatrix}$$

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(7) Suppose we have two files giving coordinates of atoms as follows:

File 1:

A1	1	2	3
A2	1	−1	0
A3	2	−1	1
A4	−1	0	1

File 2:

A1	0	0	0
A2	3	0	−3
A3	3	1	−2
A4	2	−2	−2

Show that these are the same structure (i. e. show that they can be moved to coincide).

(8) Let

$$D = \begin{bmatrix} 0 & 2 & 5 & 1 \\ 2 & 0 & 3 & 1 \\ 5 & 3 & 0 & 6 \\ 1 & 1 & 6 & 0 \end{bmatrix}$$

be the distance matrix for points $v_0, \ldots, v_3$. Find the gram matrix for vectors $v_1 - v_0$, $v_2 - v_0$, $v_3 - v_0$.

Solution:

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

(9) Write a 4×4 matrix to represent the transformation

$$TX \to R(\pi/6)X + (1, 1, 1)'.$$

FIGURE 1. The thick and thin curve together are a ribbon

Find T^{144} and show that it is a translation. What is the translation vector?
Solution: $(0, 0, 144)$

(10) Find the linking number of the two curve in the ribbon in figure 1.
Solution:

$$\mathrm{Lk} = 0$$