Sheet 08.4: Matrices III: Unitary, Orthogonal, Diagonalization

Posted: Friday, 04.12.15 Due: Monday, 14.12.15, 13:00 Central Tutorial: 16.12.15
(b)[2](E/M/A) means: problem (b) counts 2 points and is easy/medium hard/advanced
Example problems: {T}: will be discussed in tutorial; {S}: self study.

Example Problem 1: Orthogonal and unitary matrices [2]
Points: (a)[1](E); (b)[0,5](E); (c)[0,5](E). [T]

(a) Is the matrix A as given below an orthogonal matrix? Is B unitary?

$$A = \begin{pmatrix} \sin\theta & \cos\theta \\ -\cos\theta & \sin\theta \end{pmatrix}, \qquad B = \frac{1}{1-i}\begin{pmatrix} 2 & 1+\mathrm{i} & 0 \\ 1+\mathrm{i} & -1 & 1 \\ 0 & 2 & \mathrm{i} \end{pmatrix}$$

(b) Let $\mathbf{x} = (1,2)^T$. Calculate $\mathbf{a} = A\mathbf{x}$ explicitly, as well as the norm of $\mathbf{x}$ and $\mathbf{a}$. Does the action of A on $\mathbf{x}$ conserve its norm?

(c) Let $\mathbf{y} = (1,2,\mathrm{i})^T$. Calculate $\mathbf{b} = B\mathbf{y}$ explicitly, and also the norm of $\mathbf{y}$ and $\mathbf{b}$. Does the action of B on $\mathbf{y}$ conserve its norm?

Example Problem 2: Diagonalising real 2×2 matrices [3]
Points: (a)[1,5](E); (b)[1,5](E). [T]

For the following real matrices, find the eigenvalues $\lambda_j \in \mathbb{R}$, eigenvectors $\mathbf{v}_j \in \mathbb{R}^2$ and the similarity transformation S, as well as its inverse, S^{-1}, for which $S^{-1}AS$ is diagonal:

(a) $A = \begin{pmatrix} -1 & 6 \\ -2 & 6 \end{pmatrix}$, (b) $A = \frac{1}{5}\begin{pmatrix} 11 & -8 \\ -8 & -1 \end{pmatrix}$.

Example Problem 3: Diagonalising complex 2×2 matrices [3]
Points: (a)[1,5](M); (b)[1,5](M). [T]

For the following complex matrices, find the eigenvalues $\lambda_j \in \mathbb{C}$, eigenvectors $\mathbf{v}_j \in \mathbb{C}^2$ and the similarity transformation S, as well as its inverse, S^{-1}, for which $S^{-1}AS$ is diagonal:

(a) $A = \begin{pmatrix} -\mathrm{i} & 0 \\ 2 & \mathrm{i} \end{pmatrix}$, (b) $A = \begin{pmatrix} 1 & \mathrm{i} \\ -\mathrm{i} & 1 \end{pmatrix}$.

Example Problem 4: Diagonalising a matrix that depends on a variable [2]
Points: [2](M). [S]

Consider the matrix $A = \begin{pmatrix} x & 1 & 0 \\ 1 & 2 & 1 \\ 3-x & -1 & 3 \end{pmatrix}$, which depends on the variable $x \in \mathbb{R}$. Find the eigenvalues λ_j and eigenvectors $\mathbf{v}_j \in \mathbb{R}^3$ of A, with $j = 1, 2, 3$.
Hints: One of the eigenvalues is $\lambda = x$. (Of course the other results, too, can depend on x.) Avoid fully multiplying out the characteristic polynomial; try instead to directly bring it to a completely factorized form! [Check your results: for $x = 4$, two of the (unnormalized) eigenvectors are given by $(1, -2, -1)^T$ and $(1, -1, -2)^T$.]

Example Problem 5: Inertia tensor [2]
Points: [2](M). [S]

The inertia tensor of a rigid body composed of point masses is defined as

$$\widetilde{I}_{ij} = \sum_a m_a \, \widetilde{I}_{ij}(\mathbf{r}_a, \mathbf{r}_a) \; , \quad \text{mit} \quad \widetilde{I}_{ij}(\mathbf{r}, \mathbf{r}') \equiv \delta_{ij} \mathbf{r} \cdot \mathbf{r}' - (\mathbf{e}_i \cdot \mathbf{r})(\mathbf{e}_j \cdot \mathbf{r}') \; ,$$

where m_a and $\mathbf{r}_a = (r^1_{\ a}, r^2_{\ a}, r^3_{\ a})^T$ are, respectively, the mass and position of point mass a. The eigenvalues of the inertia tensor are known as the rigid body's *moments of inertia*.
Consider a rigid body consisting of three point masses $m_1 = 4$, $m_2 = M$ and $m_3 = 1$ at positions $\mathbf{r}_1 = (1, 0, 0)^T$, $\mathbf{r}_2 = (0, 1, 2)^T$ and $\mathbf{r}_3 = (0, 4, 1)^T$, respectively. Determine its inertia tensor $\widetilde{I}$ and moments of inertia as functions of M. (Eigenvectors are not required.) [Check your results: if $M = 5$, then $\lambda_1 = 42$, $\lambda_2 = 39$, $\lambda_3 = 11$.]

Example Problem 6: Degenerate Eigenvalue Problem [3]
Points: [3](A). [T]

For the matrix $A = \begin{pmatrix} 2 & -1 & 2 \\ -1 & 2 & -2 \\ 2 & -2 & 5 \end{pmatrix}$, find the eigenvalue λ_j, the normalized eigenvectors $\mathbf{v}_j \in \mathbb{R}^3$, and the similarity transformation S such that $S^{-1}AS$ is diagonal. *Hint:* One eigenvalue is $\lambda_1 = 1$. [Check your result: verify that $S^{-1}AS$ contains the eigenvalues on the diagonal.]

Example Problem 7: Determinant equals product of eigenvalues [1]
Points: [1](M). [S]

If A is an $n \times n$ matrix with eigenvalues $\lambda_1, \ldots, \lambda_n$, then $\det A = \prod_{j=1}^n \lambda_j$, i.e. the determinant is equal to the product of the eigenvalues. Prove this for the case that A is diagonalizable.

Example Problem 8: General Gaussian integrals [4]
Points: (a)[2](M); (b)[1](E); (c)[1](E). [T]

Multiple Gaussian integrals are integrals of the form

$$I = \int_{\mathbb{R}^n} \mathrm{d}x^1 \ldots \mathrm{d}x^n \, \mathrm{e}^{-\mathbf{r}^T A \mathbf{r}} \; ,$$

where $\mathbf{r} = (x^1, \ldots, x^n)^T$ and the matrix A is symmetric and positiv definite (i.e. all eigenvalues of A are > 0). The characteristic property of this class of integrals is that the exponent is a 'quadratic form', i.e. a *quadratic* function of all integration variables. In general this function contains mixed terms, but these can be removed by a basis transformation: Let S be the similarity transformation that diagonalizes A, so that $D = S^T AS$ is diagonal, with eigenvalues $\lambda_1, \ldots, \lambda_n$. Since A is symmetric, S is orthogonal, with $S^{-1} = S^T$ and $\det S = 1$. Now define $\tilde{\mathbf{r}} = (\tilde{x}^1, \dots, \tilde{x}^n)^T$ by $\tilde{\mathbf{r}} \equiv S^T \mathbf{r}$, then we have

$$\mathbf{r}^T A \mathbf{r} = \mathbf{r}^T S D S^T \mathbf{r} = \tilde{\mathbf{r}}^T D \, \tilde{\mathbf{r}} = \sum_i \lambda_i (\tilde{x}^i)^2 \, . \tag{1}$$

When expressed through the new variables $\tilde{\mathbf{r}}$, the exponent thus no longer contains any mixed terms, so that the Gaussian integral can be solved by the variable substitution $\mathbf{r} = S\tilde{\mathbf{r}}$:

$$I = \int_{\mathbb{R}^n} \mathrm{d}x^1 \dots \mathrm{d}x^n \, \mathrm{e}^{-\mathbf{r}^T A \mathbf{r}} = \int_{\mathbb{R}^n} \mathrm{d}\tilde{x}^1 \dots \mathrm{d}\tilde{x}^n \, J \, \mathrm{e}^{-\sum_i^n \lambda_n (\tilde{x}^i)^2} = \sqrt{\frac{\pi}{\lambda_1}} \cdots \sqrt{\frac{\pi}{\lambda_n}} = \boxed{\sqrt{\frac{\pi^n}{\det A}}} \, .$$

We have here exploited two facts: (i) Since $\partial x^i / \partial \tilde{x}^j = S^i_{\ j}$, the Jacobian determinant of the variable substitution equals the determinant of S and thus equal to 1:

$$J = \left| \frac{\partial(x^1, \dots, x^n)}{\partial(\tilde{x}^1, \dots, \tilde{x}^n)} \right| = \left| \det \begin{pmatrix} \frac{\partial x^1}{\partial \tilde{x}^1} & \dots & \frac{\partial x^1}{\partial \tilde{x}^n} \\ \vdots & & \vdots \\ \frac{\partial x^n}{\partial \tilde{x}^1} & \dots & \frac{\partial x^n}{\partial \tilde{x}^n} \end{pmatrix} \right| = \left| \det \begin{pmatrix} S^1_{\ 1} & \dots & S^1_{\ n} \\ \vdots & & \vdots \\ S^n_{\ 1} & \dots & S^n_{\ n} \end{pmatrix} \right| = |\det S| = 1 \, .$$

(ii) The product of the eigenvalues of a matrix equals its determinant, $\prod_i^n \lambda_i = \det A$.

Now use the above strategy to compute the following integral:

$$I = \int_{\mathbb{R}^2} \mathrm{d}x \, \mathrm{d}y \, \mathrm{e}^{-\left(2x^2 + 6xy + 10y^2\right)}$$

Execute all steps of the above argumentation explicitly:

(a) Bring the exponent into the form $-\mathbf{r}^T A \mathbf{r}$, with $\mathbf{r} = (x, y)^T$ and A symmetric. Identify and diagonalize the matrix A. In particular, explicitly write out equation (1) for the present case.

(b) Find S. Calculate the Jacobian determinant explicitly.

(c) What is the value of the Gaussian integral?

[Total Points for Example Problems: 20]

Homework Problem 1: Orthogonal and unitary matrices [2]
Points: (a)[1](E); (b)[0,5](E); (c)[0,5](E)

(a) Determine if whether the following matrices are orthogonal or unitary:

$$A = \begin{pmatrix} 0 & 3 & 0 \\ 2 & 0 & 1 \\ -1 & 0 & 2 \end{pmatrix}, \quad B = \frac{1}{3} \begin{pmatrix} 1 & 2 & -2 \\ -2 & 2 & 1 \\ 2 & 1 & 2 \end{pmatrix}, \quad C = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathrm{i} & 1 \\ -1 & -\mathrm{i} \end{pmatrix}$$

(b) Let $\mathbf{x} = (1, 2, -1)^T$. Calculate $\mathbf{a} = A\mathbf{x}$ and $\mathbf{b} = B\mathbf{x}$ explicitly. Also, calculate the norm of $\mathbf{x}$, $\mathbf{a}$ and $\mathbf{b}$. Which of these norms should be equal? Why?

(c) Let $\mathbf{y} = (1, \mathrm{i})^T$. Calculate $\mathbf{c} = C\mathbf{y}$ explicitly, and also determine the norm of $\mathbf{y}$ and $\mathbf{c}$. Should the norms be equal? Why?

Homework Problem 2: Diagonalising real 2×2 matrices [3]
Points: (a)[1,5](E); (b)[1,5](E)

For the following real matrices, find the eigenvalues $\lambda_j \in \mathbb{R}$, eigenvectors $\mathbf{v}_j \in \mathbb{R}^2$ and the similarity transformation S, as well as its inverse, S^{-1}, for which $S^{-1}AS$ is diagonal:

(a) $A = \begin{pmatrix} 4 & -6 \\ 3 & -5 \end{pmatrix}$, (b) $A = \frac{1}{10}\begin{pmatrix} -19 & 3 \\ 3 & -11 \end{pmatrix}$.

Homework Problem 3: Diagonalising complex 3×3 matrices [4]
Points: (a)[2](A); (b)[2](M)

For the following complex matrices, find the eigenvalues $\lambda_j \in \mathbb{C}$, eigenvectors $\mathbf{v}_j \in \mathbb{C}^3$ and the similarity transformation S, as well as its inverse, S^{-1}, for which $S^{-1}AS$ is diagonal:

(a) $A = \begin{pmatrix} 1 & 0 & -1 \\ 0 & 2\mathrm{i} & 0 \\ 1 & 0 & 1 \end{pmatrix}$, (b) $A = \begin{pmatrix} 1 & 0 & -\mathrm{i} \\ 0 & 1 & 0 \\ \mathrm{i} & 0 & 1 \end{pmatrix}$.

Homework Problem 4: Qubit [3]
Points: (a)[1](M); (b)[2](M)

A qubit (for "quantum bit" = quantum version of a classical bit) is a manipulable two-level quantum systems (`http://en.wikipedia.org/wiki/Qubit`). The simplest version of a qubit is described by the matrix $H = \begin{pmatrix} B & \overline{\Delta} \\ \Delta & -B \end{pmatrix}$, with $B \in \mathbb{R}$ and $\Delta \in \mathbb{C}$.

(a) Calculate the eigenvalues E_j (choose $E_1 < E_2$) and normalized eigenvectors $\mathbf{v}_1$ and $\mathbf{v}_2$ of H as a function of B, Δ and $X \equiv [B^2 + |\overline{\Delta}|^2]^{1/2}$.

(b) Show that the eigenvectors can be brought to the form $\mathbf{v}_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} -\sqrt{1-Y} \\ \mathrm{e}^{\mathrm{i}\phi}\sqrt{1+Y} \end{pmatrix}$ and $\mathbf{v}_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{1+Y} \\ \mathrm{e}^{\mathrm{i}\phi}\sqrt{1-Y} \end{pmatrix}$, where $\mathrm{e}^{\mathrm{i}\phi}$ is the phase factor of $\Delta \equiv |\Delta|\mathrm{e}^{\mathrm{i}\phi}$. How does Y scale as a function of B and X? On three diagrams arranged below each other, each showing two curves, sketch first E_1 and E_2, second, the square of the absolute values of the components $|v_1^1|^2$ and $|v_1^2|^2$ of the eigenvector $\mathbf{v}_1$, and third the square of the absolute values of the components of $|v_2^1|^2$ and $|v_2^2|^2$ of the eigenvector $\mathbf{v}_2$, all as functions of $B/|\Delta| \in \{-\infty, \infty\}$ at fixed $|\Delta|$.

Background information: The first sketch shows the so called "avoided crossing", a typical trait of a quantum bit. The second and third sketches show that the eigenvectors "exchange their roles" if B/Δ goes from $-\infty$ to $+\infty$. Both these properties have been detected in many experiments. (See for e.g. `http://www.sciencemag.org/content/299/5614/1869.abstract`, Fig. 2A und 2B.)

Homework Problem 5: Inertia tensor [2]
Points: (a)[1](E); (b)[1](E).

Consider a rigid body consisting of two point masses, $m_1 = \frac{2}{3}$ and $m_2 = 3$, at positions $\mathbf{r}_1 = (2, 2, -1)^T$ and $\mathbf{r}_2 = \frac{1}{3}(2, -1, 2)^T$, respectively.

(a) Show that its inertia tensor has the following form: $\widetilde{I} = \begin{pmatrix} 5 & -2 & 0 \\ -2 & 6 & 2 \\ 0 & 2 & 7 \end{pmatrix}$.

(b) Find the moments of inertia (eigenvalues). (Eigenvectors need not be computed.) (*Hint:* One eigenvalue is $\lambda = 3$.)

Homework Problem 6: Degenerate Eigenvalue Problem [3]
Points: (a)[3](A); (b)[3](A,Bonus)

Consider the following matrices:

$$A = \begin{pmatrix} 15 & 6 & -3 \\ 6 & 6 & 6 \\ -3 & 6 & 15 \end{pmatrix}, \qquad B = \begin{pmatrix} -1 & 0 & 0 & 2\mathrm{i} \\ 0 & 7 & 2 & 0 \\ 0 & 2 & 4 & 0 \\ -2\mathrm{i} & 0 & 0 & 2 \end{pmatrix}.$$

(a) One of the eigenvectors $\mathbf{v}_j \in \mathbb{R}^3$ of the matrix A is $\mathbf{v}_3 = \frac{1}{\sqrt{3}}(1,1,1)^T$. Find all eigenvalues λ_j of A. (*Hint:* Two eigenvalues are degenerate.) Construct an orthonormal basis $\{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3\}$ of $\mathbb{R}^3$ consisting of eigenvectorss of A. Find a similarity transformation S, and its inverse S^{-1}, for which $S^{-1}AS$ is diagonal.

(b) One of the eigenvectors $\mathbf{v}_j \in \mathbb{C}^4$ of the matrix B is $\mathbf{v}_3 = \frac{1}{\sqrt{5}}(0,1,-2,0)^T$. Find all eigenvalues λ_j of B. (*Hint:* Two eigenvalues are degenerate.) Construct an orthonormal basis $\{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3, \mathbf{v}_4\}$ of $\mathbb{C}^4$ consisting of eigenvectors of B. Find a similarity transformation S, and its inverse S^{-1}, for which $S^{-1}BS$ is diagonal.

Homework Problem 7: Spur einer Matrix [2]
Points: (a)[0,5](M); (b)[0,5](M); (c)[1](M)

The trace of an $n\times n$ matrix, $\mathrm{Tr}\, A$, is defined as the sum of all diagonal elements, $\mathrm{Tr}\, A = \sum_{j=1}^{n} A_{jj}$. Show the following properties of the trace:

(a) $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$ for any $n \times n$ matrices A and B.

(b) $\mathrm{A} = \mathrm{Tr}(S^{-1}AS)$ for any $n \times n$ matrices A and S, where S is invertible.

(c) If A has the eigenvalues $\lambda_1, \ldots, \lambda_n$, then $\mathrm{Tr}\, A = \lambda_1 + \ldots + \lambda_n$. You may assume that A is diagonalizable.

Homework Problem 8: Three-dimensional Gaussian integral with mixed terms in the exponent [3]
Points: (a)[1](M); (b)[1](M); (c)[1](M)

Compute the following three-dimensional Gaussian integral:

$$I = \int_{\mathbb{R}^3} \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}z\, \mathrm{e}^{-\left(5x^2+5y^2+5z^2+8xy+8yz+8xz\right)}$$

(a) Bring the exponent into the form $-\mathbf{r}^T A \mathbf{r}$, with $\mathbf{r} = (x,y,z)^T$ and A symmetrical.

(b) Diagonalize the matrix A. You do not need to compute the corresponding similarity transformation explicitly.

(c) Compute I by expressing it as a product of three one-dimensional Gaussian integrals.

[Total Points for Homework Problems: 22]
