Sheet 08: Matrices III: Unitary, Orthogonal, Diagonalization

Posted: Mo 06.12.21 Central Tutorial: Do 09.12.21 Due: Th 16.12.21, 14:00
(b)[2](E/M/A) means: problem (b) counts 2 points and is easy/medium hard/advanced
Suggestions for central tutorial: example problems 2, 5, 6.
Videos exist for example problems 2 (L7.3.1), 6 (C4.5.5).

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

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

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

(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: Matrix diagonalization [4]
Points: (a)[1](E); (a)[1](E); (c)[2](E).

For each of the following matrices, find the eigenvalues λ_j and a set of eigenvectors $\mathbf{v}_j$. Also find a similarity transformation, T, and its inverse, T^{-1}, for which $T^{-1}AT$ is diagonal.

(a) $A = \begin{pmatrix} -1 & 6 \\ -2 & 6 \end{pmatrix}$, (b) $A = \begin{pmatrix} -\mathrm{i} & 0 \\ 2 & \mathrm{i} \end{pmatrix}$ (c) $A = \begin{pmatrix} 1 & 0 & -1 \\ 0 & 2\mathrm{i} & 0 \\ 1 & 0 & 1 \end{pmatrix}$.

[Consistency checks: Do the eigenvalues satisfy $\sum_j \lambda_j = \mathrm{Tr}\, A$ and $\prod_j \lambda_j = \det A$? Does $T^{-1}AT$ yield a matrix, $D = \mathrm{diag}\{\lambda_j\}$, containing the eigenvalues on the diagonal, or conversely, does TDT^{-1} reproduce A? Which of the latter two checks do you find more efficient?]

Example Problem 3: Diagonalizing symmetric or Hermitian matrices [4]
Points: (a)[1](E); (a)[1](E); (c)[2](E).

For each of the following matrices, find the eigenvalues λ_j and a set of eigenvectors $\mathbf{v}_j$. Also find a similarity transformation, T, and its inverse, T^{-1}, for which $T^{-1}AT$ is diagonal.

(a) $A = \begin{pmatrix} 3 & -4 \\ -4 & -3 \end{pmatrix}$, (b) $A = \begin{pmatrix} 1 & \mathrm{i} \\ -\mathrm{i} & 1 \end{pmatrix}$, (c) $A = \begin{pmatrix} 1 & 0 & -\mathrm{i} \\ 0 & 1 & 0 \\ \mathrm{i} & 0 & 1 \end{pmatrix}$.

Hint: Each of these matrices is either symmetric or Hermitian. Therefore T can respectively be chosen to be either orthogonal or unitary, which facilitates computing its inverse using $T^{-1} = T^T$ or $T^{-1} = T^\dagger$. To achieve this, the columns of T, containing the eigenvectors $\mathbf{v}_j$, must form an orthonormal system w.r.t. to the real or complex scalar product, respectively. It is therefore advisable to normalize all eigenvectors as $\|\mathbf{v}_j\| = 1$. Moreover, recall that non-degenerate eigenvectors of symmetric or Hermitian matrices are guaranteed to be orthogonal.

[Consistency checks: Do the sum and the product of all eigenvalues yield $\mathrm{Tr}(A)$ and $\det(A)$, respectively? Let D be the diagonal matrix containing all eigenvalues; does TDT^{-1} yield A?]

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

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 as functions of x, 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: Degenerate eigenvalue problem [3]
Points: [3](A).

Consider the the matrix $A = \begin{pmatrix} 2 & -1 & 2 \\ -1 & 2 & -2 \\ 2 & -2 & 5 \end{pmatrix}$.
Find its eigenvalues λ_j, a set of *orthonormal* eigenvectors $\mathbf{v}_j$, and a similarity transformation T, as well as its inverse, T^{-1}, such that $T^{-1}AT$ is diagonal. *Hint:* One eigenvalue is $\lambda_1 = 1$.
[Consistency checks: Do the sum and the product of all eigenvalues yield $\mathrm{Tr}(A)$ and $\det(A)$, respectively? Let D be the diagonal matrix containing all eigenvalues; does TDT^{-1} yield A?]

Example Problem 6: Multi-dimensional Gaussian integrals [4]
Points: (a)[2](M); (b)[1](E); (c)[1](E).

Multiple Gaussian integrals are integrals of the form

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

where $\mathbf{x} = (x^1, ..., x^n)^T$ and the matrix A is symmetric and positive 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 T be the similarity transformation that diagonalizes A, so that $D = T^{-1}AT$ is diagonal, with eigenvalues $\lambda_1, ..., \lambda_n$. Since A is symmetric, T can be chosen orthogonal, with $T^{-1} = T^T$ and $\det T = 1$. Now define $\tilde{\mathbf{x}} = (\tilde{x}^1, ..., \tilde{x}^n)^T$ by $\tilde{\mathbf{x}} \equiv T^T \mathbf{x}$, then we have

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

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

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

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

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

(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 ($a > 0$):

$$I(a) = \int_{\mathbb{R}^2} \mathrm{d}x \, \mathrm{d}y \, \mathrm{e}^{-\left[(a+3)x^2 + 2(a-3)xy + (a+3)y^2\right]}$$

Execute all steps of the above argumentation explicitly:

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

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

(c) What is the value of the Gaussian integral? [Check your result: $I(1) = \frac{\pi}{2\sqrt{3}}$.]

Example Problem 7: Spin-$\frac{1}{2}$ matrices: eigenvalues and eigenvectors [Bonus]
Points: [3](Bonus,E).

The following matrices are used to describe quantum mechanical particles with spin $\frac{1}{2}$:

$$S_x = \tfrac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad S_y = \tfrac{1}{2} \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \qquad S_z = \tfrac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} .$$

For each matrix S_j ($j = x, y, z$), compute its two eigenvalues $\lambda_{j,a}$ and normalized eigenvectors $\mathbf{v}_{j,a}$ ($a = 1, 2$). Choose the phase of the eigenvector normalization factor in such a way that the 1-component, $v^1_{\ j,a}$ (or, if it vanishes, the 2-component), is positive and real.
[Check your results: all three matrices have the same eigenvalues, and $\sum_{a=1}^2 \lambda_{j,a} = 0$.]

[Total Points for Example Problems: 19]

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: Matrix diagonalization [4]
Points: (a)[1](E); (a)[1](E); (c)[2](E).

For each of the following matrices, find the eigenvalues λ_j and a set of eigenvectors $\mathbf{v}_j$. For definiteness, choose the first element of each eigenvector equal to unity, $\mathbf{v}^1_{\ j} = 1$. Find a similarity transformation, T, and its inverse, T^{-1}, for which $T^{-1}AT$ is diagonal.

(a) $A = \begin{pmatrix} 4 & -6 \\ 3 & -5 \end{pmatrix}$, (b) $A = \begin{pmatrix} 2-\mathrm{i} & 1+\mathrm{i} \\ 2+2\mathrm{i} & -1+2\mathrm{i} \end{pmatrix}$ (c) $A = \begin{pmatrix} -1 & 1 & 0 \\ 1 & 1 & 1 \\ 3 & -1 & 2 \end{pmatrix}$.

[Consistency checks: Do the sum and the product of all eigenvalues yield $\mathrm{Tr}(A)$ and $\det(A)$, respectively? Let D be the diagonal matrix containing all eigenvalues; does TDT^{-1} yield A?]

Homework Problem 3: Diagonalizing symmetric or Hermitian matrices [4]
Points: (a)[1](E); (a)[1](E); (c)[2](E).

For each of the following matrices, find the eigenvalues λ_j and a set of eigenvectors $\mathbf{v}_j$. Also find a similarity transformation, T, and its inverse, T^{-1}, for which $T^{-1}AT$ is diagonal.

(a) $A = \frac{1}{10}\begin{pmatrix} -19 & 3 \\ 3 & -11 \end{pmatrix}$, (b) $A = \begin{pmatrix} 0 & 1 & 0 \\ 1 & -1 & 1 \\ 0 & 1 & 0 \end{pmatrix}$, (c) $A = \begin{pmatrix} 1 & \mathrm{i} & 0 \\ -\mathrm{i} & 2 & -\mathrm{i} \\ 0 & \mathrm{i} & 1 \end{pmatrix}$.

[Consistency checks: Do the sum and the product of all eigenvalues yield $\mathrm{Tr}(A)$ and $\det(A)$, respectively? Let D be the diagonal matrix containing all eigenvalues; does TDT^{-1} yield A?]

Homework Problem 4: Diagonalizing a matrix depending on two variables: 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 $X \equiv [B^2 + |\Delta|^2]^{1/2}$.

(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 depend on B and X? On three diagrams arranged below each other, each showing two curves, sketch first E_1 and E_2, second $|v^1_{\ 1}|^2$ and $|v^2_{\ 1}|^2$, the squares of the absolute values of the components of the eigenvector $\mathbf{v}_1$, and third $|v^1_{\ 2}|^2$ and $|v^2_{\ 2}|^2$, the squares of the absolute values of the components of of the eigenvector $\mathbf{v}_2$, all as functions of $B/|\Delta| \in \{-\infty, \infty\}$ for 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 and 2B.)

Homework Problem 5: Degenerate eigenvalue problem [3]
Points: (a)[3](A); (b)[3](A,Bonus)

For each of the following matrices, find the eigenvalues λ_j, a set of *orthonormal* eigenvectors $\mathbf{v}_j$, and a similarity transformation, T, and its inverse, T^{-1}, for which $T^{-1}AT$ is diagonal.

$$\text{(a)}\;\; A = \begin{pmatrix} 15 & 6 & -3 \\ 6 & 6 & 6 \\ -3 & 6 & 15 \end{pmatrix}, \qquad \text{(b)}\;\; A = \begin{pmatrix} -1 & 0 & 0 & 2\mathrm{i} \\ 0 & 7 & 2 & 0 \\ 0 & 2 & 4 & 0 \\ -2\mathrm{i} & 0 & 0 & 2 \end{pmatrix}.$$

Hints: Both these matrices have a pair of degenerate eigenvalues. Call these $\lambda_2 = \lambda_3$. One of the corresponding eigenvectors is $\mathbf{v}_3 = \frac{1}{\sqrt{3}}(1,1,1)^T$ for (a) and $\mathbf{v}_3 = \frac{1}{\sqrt{5}}(0,1,-2,0)^T$ for (b).
[Consistency checks: Do the sum and the product of all eigenvalues yield $\mathrm{Tr}(A)$ and $\det(A)$, respectively? Let D be the diagonal matrix containing all eigenvalues; does TDT^{-1} yield A?]

Homework Problem 6: 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 ($a > 0$):

$$I(a) = \int_{\mathbb{R}^3} \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{e}^{-\left[(a+2)x^2+(a+2)y^2+(a+2)z^2+2(a-1)xy+2(a-1)yz+2(a-1)xz\right]}$$

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

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

(c) Compute $I(a)$ by expressing it as a product of three one-dimensional Gaussian integrals. [Check your result: $I(3) = \frac{1}{9}\sqrt{\pi^3}$.]

Homework Problem 7: Spin-1 matrices: eigenvalues and eigenvectors [Bonus]
Points: [3](Bonus,E).

The following matrices are used to describe quantum mechanical particles with spin 1:

$$S_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \qquad S_y = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -\mathrm{i} & 0 \\ \mathrm{i} & 0 & -\mathrm{i} \\ 0 & \mathrm{i} & 0 \end{pmatrix}, \quad S_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

For each matrix S_j ($j = x,y,z$), compute its three eigenvalues $\lambda_{j,a}$ and normalized eigenvectors $\mathbf{v}_{j,a}$ ($a = 1,2,3$). Choose the phase of the eigenvector normalization factor in such a way that the 1-component, $v^1_{j,a}$ (or, if it vanishes, the 2- or 3-component), is positive and real.

[Check your results: all three matrices have the same eigenvalues, and $\sum_{a=1}^{3} \lambda_{j,a} = 0$.]

[Total Points for Homework Problems: 19]