# Sheet 08: Matrices III: Unitary, Orthogonal, Diagonalization

Posted: Mo 05.12.22 Central Tutorial: Do 08.12.22 Due: Th 15.12.22, 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 $\lambda_j$ 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 $\lambda_j$ 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 $\lambda_j$ 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 $\lambda_j$, 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

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

where $\mathbf{x} = (x^1, \ldots, x^n)^T$ 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 $\lambda_1, \ldots, \lambda_n$. Since $A$ is symmetric, $T$ can be chosen orthogonal, with $T^{-1} = T^T$ and $\det T = 1$. Now define $\tilde{\mathbf{x}} = (\tilde{x}^1, \ldots, \tilde{x}^n)^T$ by $\tilde{\mathbf{x}} \equiv T^T \mathbf{x}$, then we have

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

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 $\frac{1}{2}$:

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

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 $\sum_{a=1}^2 \lambda_{j,a} = 0$.]

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[Total Points for Example Problems: 19]

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**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 $\lambda_j$ 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 $\lambda_j$ 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 $B$, $\Delta$ 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 $B/\Delta$ 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 $\lambda_j$, 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.

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

*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 $\sum_{a=1}^{3} \lambda_{j,a} = 0$.]

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[Total Points for Homework Problems: 19]

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