Basis changes and matrix diagonalization

1. Coordinates of vectors and matrix elements of linear operators

Let V be an n-dimensional real (or complex) vector space. Vectors that live in V are usually represented by a single column of n real (or complex) numbers. Linear operators act on vectors and are represented by square $n \times n$ real (or complex) matrices.*

If it is not specified, the representations of vectors and matrices described above implicitly assume that the *standard basis* has been chosen. That is, all vectors in V can be expressed as linear combinations of basis vectors:

$$\begin{aligned}\mathcal{B}_s &= \left\{\widehat{\boldsymbol{e}}_1\,,\,\widehat{\boldsymbol{e}}_2\,,\,\widehat{\boldsymbol{e}}_3\,,\,\ldots\,,\,\widehat{\boldsymbol{e}}_n\right\} \\ &= \left\{(1,0,0,\ldots,0)^{\mathsf{T}}\,,\,(0,1,0,\ldots,0)^{\mathsf{T}}\,,\,(0,0,1,\ldots,0)^{\mathsf{T}}\,,\,\ldots\,,\,(0,0,0,\ldots,1)^{\mathsf{T}}\right\}.\end{aligned}$$

The subscript s indicates that this is the standard basis. The superscript T (which stands for *transpose*) turns the row vectors into column vectors. Thus,

$$\vec{\boldsymbol{v}} = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \\ v_n \end{pmatrix} = v_1 \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + v_2 \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ v_n \end{pmatrix} + v_3 \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix} + \cdots + v_n \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}.$$

The v_i are the components of the vector $\vec{\boldsymbol{v}}$. However, it is more precise to say that the v_i are the *coordinates* of the abstract vector $\vec{\boldsymbol{v}}$ with respect to the standard basis.

Consider a linear operator A. The corresponding matrix representation is given by $A = [a_{ij}]$. For example, if $\vec{\boldsymbol{w}} = A\vec{\boldsymbol{v}}$, then

$$w_i = \sum_{j=1}^{n} a_{ij} v_j \,, \tag{1}$$

where v_i and w_i are the coordinates of $\vec{\boldsymbol{v}}$ and $\vec{\boldsymbol{w}}$ with respect to the standard basis and a_{ij} are the matrix elements of A with respect to the standard basis. If we express

*A linear operator is a function that acts on vectors that live in a vector space V over a field F and produces a vector that lives in another vector space W. If V is n-dimensional and W is m-dimensional, then the linear operator is represented by an $m \times n$ matrix, whose entries are taken from the field F. Typically, we choose either $F = \mathbb{R}$ (the real numers) or $F = \mathbb{C}$ (the complex numbers). In these notes, we will simplify the discussion by always taking $W = V$.

$\vec{\boldsymbol{v}}$ and $\vec{\boldsymbol{w}}$ as linear combinations of basis vectors, then

$$\vec{\boldsymbol{v}} = \sum_{j=1}^{n} v_j \widehat{\boldsymbol{e}}_j\,, \qquad\qquad \vec{\boldsymbol{w}} = \sum_{i=1}^{n} w_i \widehat{\boldsymbol{e}}_i\,,$$

then $\vec{\boldsymbol{w}} = A\vec{\boldsymbol{v}}$ implies that

$$\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij} v_j \widehat{\boldsymbol{e}}_i = A \sum_{j=1}^{n} v_j \widehat{\boldsymbol{e}}_j\,,$$

where we have used eq. (1) to substitute for w_i. It follows that:

$$\sum_{j=1}^{n}\left(A\widehat{\boldsymbol{e}}_j - \sum_{i=1}^{n} a_{ij}\widehat{\boldsymbol{e}}_i\right) v_j = 0\,. \tag{2}$$

Eq. (2) must be true for *any* vector $\vec{\boldsymbol{v}} \in V$; that is, for any choice of coordinates v_j. Thus, the coefficient inside the parentheses in eq. (2) must vanish. We conclude that:

$$\boxed{A\widehat{\boldsymbol{e}}_j = \sum_{i=1}^{n} a_{ij}\widehat{\boldsymbol{e}}_i} \tag{3}$$

which can be used as the definition of the matrix elements a_{ij} with respect to the standard basis of a linear operator A.

There is nothing sacrosanct about the choice of the standard basis. One can expand a vector as a linear combination of any set of n linearly independent vectors. Thus, we generalize the above discussion by introducing a basis

$$\mathcal{B} = \left\{\vec{\boldsymbol{b}}_1\,,\, \vec{\boldsymbol{b}}_2\,,\, \vec{\boldsymbol{b}}_3\,,\, \ldots\,,\, \vec{\boldsymbol{b}}_n\right\}.$$

For any vector $\vec{\boldsymbol{v}} \in V$, we can find a unique set of coefficients v_i such that

$$\vec{\boldsymbol{v}} = \sum_{j=1}^{n} v_j\, \vec{\boldsymbol{b}}_j\,. \tag{4}$$

The v_i are the *coordinates* of $\vec{\boldsymbol{v}}$ with respect to the basis $\mathcal{B}$. Likewise, for any linear operator A,

$$A\vec{\boldsymbol{b}}_j = \sum_{i=1}^{n} a_{ij}\vec{\boldsymbol{b}}_i \tag{5}$$

defines the *matrix elements* of the linear operator A with respect to the basis $\mathcal{B}$. Clearly, these more general definitions reduce to the previous ones given in the case of the standard basis. Moreover, we can easily compute $A\vec{\boldsymbol{v}} \equiv \vec{\boldsymbol{w}}$ using the results of eqs. (4) and (5):

$$A\vec{\boldsymbol{v}} = \sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij} v_j \vec{\boldsymbol{b}}_i = \sum_{i=1}^{n}\left(\sum_{j=1}^{n} a_{ij} v_j\right)\vec{\boldsymbol{b}}_i = \sum_{i=1}^{n} w_i \vec{\boldsymbol{b}}_i = \vec{\boldsymbol{w}}\,,$$

which implies that the coordinates of the vector $\vec{\boldsymbol{w}} = A\vec{\boldsymbol{v}}$ with respect to the basis $\mathcal{B}$ are given by:

$$w_i = \sum_{j=1}^{n} a_{ij} v_j\,.$$

Thus, the relation between the coordinates of $\vec{\boldsymbol{v}}$ and $\vec{\boldsymbol{w}}$ with respect to the basis $\mathcal{B}$ is the same as the relation obtained with respect to the standard basis [see eq. (1)]. One must simply be consistent and always employ the *same* basis for defining the vector coordinates and the matrix elements of a linear operator.

2. Change of basis and its effects on coordinates and matrix elements

The choice of basis is arbitrary. The existence of vectors and linear operators does not depend on the choice of basis. However, a choice of basis is very convenient since it permits explicit calculations involving vectors and matrices. Suppose we start with some basis choice $\mathcal{B}$ and then later decide to employ a different basis choice $\mathcal{C}$:

$$\mathcal{C} = \left\{\vec{\boldsymbol{c}}_1\,,\,\vec{\boldsymbol{c}}_2\,,\,\vec{\boldsymbol{c}}_3\,,\,\ldots\,,\,\vec{\boldsymbol{c}}_n\right\}.$$

Note that we have not yet introduced the concept of an inner product or norm, so in the present discussion there is no concept of orthogonality or unit vectors. (The inner product will be employed only in Section 4 of these notes.)

Thus, we pose the following question. If the coordinates of a vector $\vec{\boldsymbol{v}}$ and the matrix elements of a linear operator A are known with respect to a basis $\mathcal{B}$ (which need not be the standard basis), what are the coordinates of the vector $\vec{\boldsymbol{v}}$ and the matrix elements of a linear operator A with respect to a basis $\mathcal{C}$? To answer this question, we must describe the relation between $\mathcal{B}$ and $\mathcal{C}$. The basis vectors of $\mathcal{C}$ can be expressed as linear combinations of the basis vectors $\vec{\boldsymbol{b}}_i$, since the latter span the vector space V. We shall denote these coefficients as follows:

$$\vec{\boldsymbol{c}}_j = \sum_{i=1}^{n} P_{ij}\vec{\boldsymbol{b}}_i\,, \qquad j = 1, 2, 3, \ldots, n\,. \tag{6}$$

Note that eq. (6) is a shorthand for n separate equations, and provides the coefficients P_{i1}, P_{i2}, …, P_{in} needed to expand $\vec{\boldsymbol{c}}_1$, $\vec{\boldsymbol{c}}_2$, …, $\vec{\boldsymbol{c}}_n$, respectively, as linear combinations of the $\vec{\boldsymbol{b}}_i$. We can assemble the P_{ij} into a matrix. A crucial observation is that this matrix P is invertible. This must be true, since one can reverse the process and express the basis vectors of $\mathcal{B}$ as linear combinations of the basis vectors $\vec{\boldsymbol{c}}_i$ (which again follows from the fact that the latter span the vector space V). Explicitly,

$$\vec{\boldsymbol{b}}_k = \sum_{j=1}^{n} (P^{-1})_{jk} \vec{\boldsymbol{c}}_j \,, \qquad k = 1, 2, 3, \ldots, n \,. \tag{7}$$

We are now in the position to determine the coordinates of a vector $\vec{\boldsymbol{v}}$ and the matrix elements of a linear operator A with respect to a basis $\mathcal{C}$. Assume that the coordinates of $\vec{\boldsymbol{v}}$ with respect to $\mathcal{B}$ are given by v_i and the matrix elements of A with respect to $\mathcal{B}$ are given by a_{ij}. With respect to $\mathcal{C}$, we shall denote the vector coordinates by v'_i and the matrix elements by a'_{ij}. Then, using the definition of vector coordinates [eq. (4)] and matrix elements [eq. (5)],

$$\vec{\boldsymbol{v}} = \sum_{j=1}^{n} v'_j \vec{\boldsymbol{c}}_j = \sum_{j=1}^{n} v'_j \sum_{i=1}^{n} P_{ij} \vec{\boldsymbol{b}}_i = \sum_{i=1}^{n} \left(\sum_{j=1}^{n} P_{ij} v'_j \right) \vec{\boldsymbol{b}}_i = \sum_{i=1}^{n} v_i \vec{\boldsymbol{b}}_i \,, \tag{8}$$

where we have used eq. (6) to express the $\vec{\boldsymbol{c}}_j$ in terms of the $\vec{\boldsymbol{b}}_i$. The last step in eq. (8) can be rewritten as:

$$\sum_{i=1}^{n} \left(v_i - \sum_{j=1}^{n} P_{ij} v'_j \right) \vec{\boldsymbol{b}}_i = 0 \,. \tag{9}$$

Since the $\vec{\boldsymbol{b}}_i$ are linearly independent, the coefficient inside the parentheses in eq. (9) must vanish. Hence,

$$v_i = \sum_{j=1}^{n} P_{ij} v'_j \,, \qquad \text{or equivalently} \qquad \boxed{[\vec{\boldsymbol{v}}]_{\mathcal{B}} = P[\vec{\boldsymbol{v}}]_{\mathcal{C}}} \,. \tag{10}$$

Here we have introduced the notation $[\vec{\boldsymbol{v}}]_{\mathcal{B}}$ to indicate the vector $\vec{\boldsymbol{v}}$ represented in terms of its coordinates with respect to the basis $\mathcal{B}$. Inverting this result yields:

$$v'_j = \sum_{k=1}^{n} (P^{-1})_{jk} v_k \,, \qquad \text{or equivalently} \qquad \boxed{[\vec{\boldsymbol{v}}]_{\mathcal{C}} = P^{-1}[\vec{\boldsymbol{v}}]_{\mathcal{B}}} \,. \tag{11}$$

Thus, we have determined the relation between the coordinates of $\vec{\boldsymbol{v}}$ with respect to the bases $\mathcal{B}$ and $\mathcal{C}$.

A similar computation can determine the relation between the matrix elements of A with respect to the basis $\mathcal{B}$, which we denote by a_{ij} [see eq. (5)], and the matrix elements of A with respect to the basis $\mathcal{C}$, which we denote by a'_{ij}:

$$A\vec{\boldsymbol{c}}_j = \sum_{i=1}^{n} a'_{ij} \vec{\boldsymbol{c}}_i \,. \tag{12}$$

The desired relation can be obtained by evaluating $A\vec{\boldsymbol{b}}_\ell$:

$$\begin{aligned}
A\vec{\boldsymbol{b}}_\ell &= A\sum_{j=1}^n (P^{-1})_{j\ell}\vec{\boldsymbol{c}}_j = \sum_{j=1}^n (P^{-1})_{j\ell}\, A\vec{\boldsymbol{c}}_j = \sum_{j=1}^n (P^{-1})_{j\ell}\sum_{i=1}^n a'_{ij}\vec{\boldsymbol{c}}_i \\
&= \sum_{j=1}^n (P^{-1})_{j\ell}\sum_{i=1}^n a'_{ij}\sum_{k=1}^n P_{ki}\vec{\boldsymbol{b}}_k = \sum_{k=1}^n\left(\sum_{i=1}^n\sum_{j=1}^n P_{ki}a'_{ij}(P^{-1})_{j\ell}\right)\vec{\boldsymbol{b}}_k\,,
\end{aligned}$$

where we have used eqs. (6) and (7) and the definition of the matrix elements of A with respect to the basis $\mathcal{C}$ [eq. (12)]. Comparing this result with eq. (5), it follows that

$$\sum_{k=1}^n\left(a_{k\ell} - \sum_{i=1}^n\sum_{j=1}^n P_{ki}a'_{ij}(P^{-1})_{j\ell}\right)\vec{\boldsymbol{b}}_k = 0\,.$$

Since the $\vec{\boldsymbol{b}}_k$ are linearly independent, we conclude that

$$a_{k\ell} = \sum_{i=1}^n\sum_{j=1}^n P_{ki}a'_{ij}(P^{-1})_{j\ell}\,.$$

The double sum above corresponds to the matrix multiplication of three matrices, so it is convenient to write this result symbolically as:

$$\boxed{[A]_\mathcal{B} = P[A]_\mathcal{C}P^{-1}\,.} \tag{13}$$

The meaning of this equation is that the matrix formed by the matrix elements of A with respect to the basis $\mathcal{B}$ is related to the matrix formed by the matrix elements of A with respect to the basis $\mathcal{C}$ by the *similarity transformation* given by eq. (13). We can invert eq. (13) to obtain:

$$\boxed{[A]_\mathcal{C} = P^{-1}[A]_\mathcal{B}P\,.} \tag{14}$$

In fact, there is a much faster method to derive eqs. (13) and (14). Consider the equation $\vec{\boldsymbol{w}} = A\vec{\boldsymbol{v}}$ evaluated with respect to bases $\mathcal{B}$ and $\mathcal{C}$, respectively:

$$[\vec{\boldsymbol{w}}]_\mathcal{B} = [A]_\mathcal{B}[\vec{\boldsymbol{v}}]_\mathcal{B}\,, \qquad\qquad [\vec{\boldsymbol{w}}]_\mathcal{C} = [A]_\mathcal{C}[\vec{\boldsymbol{v}}]_\mathcal{C}\,.$$

Using eq. (10), $[\vec{\boldsymbol{w}}]_\mathcal{B} = [A]_\mathcal{B}[\vec{\boldsymbol{v}}]_\mathcal{B}$ can be rewritten as:

$$P[\vec{\boldsymbol{w}}]_\mathcal{C} = [A]_\mathcal{B}P[\vec{\boldsymbol{v}}]_\mathcal{C}\,.$$

Hence,

$$[\vec{\boldsymbol{w}}]_\mathcal{C} = [A]_\mathcal{C}[\vec{\boldsymbol{v}}]_\mathcal{C} = P^{-1}[A]_\mathcal{B}P[\vec{\boldsymbol{v}}]_\mathcal{C}\,.$$

It then follows that

$$\left\{[A]_\mathcal{C} - P^{-1}[A]_\mathcal{B}P\right\}[\vec{\boldsymbol{v}}]_\mathcal{C} = 0\,. \tag{15}$$

Since this equation must be true for all $\vec{\boldsymbol{v}} \in V$ (and thus for any choice of $[\vec{\boldsymbol{v}}]_{\mathcal{C}}$), it follows that the quantity inside the parentheses in eq. (15) must vanish. This yields eq. (14).

The significance of eq. (14) is as follows. If two matrices are related by a similarity transformation, then these matrices may represent the *same* linear operator with respect to two different choices of basis.† These two choices are related by eq. (6). Likewise, given two matrix representations of a group G that are related by a fixed similarity transformation,

$$D_2(g) = P^{-1} D_1(g) P\,, \qquad \text{for all } g \in G\,,$$

where P is *independent* of the group element g, then we call $D_1(g)$ and $D_2(g)$ *equivalent representations*, since $D_1(g)$ and $D_2(g)$ can be regarded as matrix representations of the *same* linear operator $D(g)$ with respect to two different basis choices.

3. Application to matrix diagonalization

Consider a matrix $A \equiv [A]_{\mathcal{B}_s}$, whose matrix elements are defined with respect to the standard basis, $\mathcal{B}_s = \left\{\widehat{\boldsymbol{e}}_1\,, \widehat{\boldsymbol{e}}_2\,, \widehat{\boldsymbol{e}}_3\,, \ldots\,, \widehat{\boldsymbol{e}}_n\right\}$. The eigenvalue problem for the matrix A consists of finding all complex λ_i such that

$$A\vec{\boldsymbol{v}}_j = \lambda_j \vec{\boldsymbol{v}}_j\,, \qquad \vec{\boldsymbol{v}}_j \neq 0 \quad \text{for} \quad j = 1, 2, \ldots, n\,. \tag{16}$$

The λ_i are the roots of the characteristic equation $\det(A - \lambda\mathbf{I}) = 0$. This is an nth order polynomial equation which has n (possibly complex) roots, although some of the roots could be degenerate. If the roots are non-degenerate, then the matrix A is called *simple*. In this case, the n eigenvectors are linearly independent and span the vector space V.‡ If some of the roots are degenerate, then the corresponding n eigenvectors may or may not be linearly independent. In general, if A possesses n linearly independent eigenvectors, then A is called *semi-simple*.§ If some of the eigenvalues of A are degenerate and its eigenvectors do *not* span the vector space V, then we say that A is *defective*. A is diagonalizable if and only if it is semi-simple.¶

Since the eigenvectors of a semi-simple matrix A span the vector space V, we may define a new basis made up of the eigenvectors of A, which we shall denote by

†However, it would *not* be correct to conclude that two matrices that are related by a similarity transformation cannot represent different linear operators. In fact, one could also interpret these two matrices as representing (with respect to the *same* basis) two different linear operators that are related by a similarity transformation. That is, given two linear operators A and B and an invertible linear operator P, it is clear that if $B = P^{-1}AP$ then the matrix elements of A and B with respect to a fixed basis are related by the same similarity transformation.

‡This result is proved in the appendix to these notes.

§Note that if A is semi-simple, then A is also simple only if the eigenvalues of A are distinct.

¶The terminology, simple (semi-simple), used above should not be confused with the corresponding terminology employed to described groups that possess no proper normal (abelian) subgroups.

$\mathcal{C} = \{\vec{\boldsymbol{v}}_1\,,\, \vec{\boldsymbol{v}}_2\,,\, \vec{\boldsymbol{v}}_3\,,\, \ldots\,,\, \vec{\boldsymbol{v}}_n\}$. The matrix elements of A with respect to the basis $\mathcal{C}$, denoted by $[A]_{\mathcal{C}}$, is obtained by employing eq. (12):

$$A\vec{\boldsymbol{v}}_j = \sum_{i=1}^{n} a'_{ij}\vec{\boldsymbol{v}}_i\,.$$

But, eq. (16) implies that $a'_{ij} = \lambda_j \delta_{ij}$ (no sum over j). That is,

$$[A]_{\mathcal{C}} = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix}.$$

The relation between A and $[A]_{\mathcal{C}}$ can be obtained from eq. (14). Thus, we must determine the matrix P that governs the relation between $\mathcal{B}_s$ and $\mathcal{C}$ [eq. (6)]. Consider the coordinates of $\vec{\boldsymbol{v}}_j$ with respect to the standard basis $\mathcal{B}_s$:

$$\vec{\boldsymbol{v}}_j = \sum_{i=1}^{n} (\vec{\boldsymbol{v}}_j)_i\,\widehat{\boldsymbol{e}}_i = \sum_{i=1}^{n} P_{ij}\widehat{\boldsymbol{e}}_i\,, \tag{17}$$

where $(\vec{\boldsymbol{v}}_j)_i$ is the ith coordinate of the jth eigenvector. Using eq. (17), we identify $P_{ij} = (\vec{\boldsymbol{v}}_j)_i$. In matrix form,

$$P = \begin{pmatrix} (v_1)_1 & (v_2)_1 & \cdots & (v_n)_1 \\ (v_1)_2 & (v_2)_2 & \cdots & (v_n)_2 \\ \vdots & \vdots & \ddots & \vdots \\ (v_1)_n & (v_2)_n & \cdots & (v_n)_n \end{pmatrix}.$$

Finally, we use eq. (14) to conclude that $[A]_{\mathcal{C}} = P^{-1}[A]_{\mathcal{B}_s}P$. If we denote the diagonalized matrix by $D \equiv [A]_{\mathcal{C}}$ and the matrix A with respect to the standard basis by $A \equiv [A]_{\mathcal{B}_s}$, then

$$P^{-1}AP = D\,, \tag{18}$$

where P is the matrix whose columns are the eigenvectors of A and D is the diagonal matrix whose diagonal elements are the eigenvalues of A. Thus, we have succeeded in diagonalizing an arbitrary semi-simple matrix.

If the eigenvectors of A do *not* span the vector space V (*i.e.*, A is defective), then A is not diagonalizable.[‖] That is, there does not exist a matrix P and a diagonal matrix D such that eq. (18) is satisfied.

[‖]The simplest example of a defective matrix is $B = \left(\begin{smallmatrix} 0 & 1 \\ 0 & 0 \end{smallmatrix}\right)$. One can quickly check that the eigenvalues of B are given by the double root $\lambda = 0$ of the characteristic equation. However, solving the eigenvalue equation, $B\vec{\boldsymbol{v}} = 0$, yields only one linearly independent eigenvector, $\left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)$. One can verify explicitly that no matrix P exists such that $P^{-1}BP$ is diagonal.

4. Diagonalization by a unitary similarity transformation

Nothing in Sections 1–3 requires the existence of an inner product. However, if an inner product is defined, then the vector space V is promoted to an inner product space. In this case, we can define the concepts of orthogonality and orthonormality. In particular, given an arbitrary basis $\mathcal{B}$, we can use the Gram-Schmidt process to construct an orthonormal basis. Thus, when considering inner product spaces, it is convenient to always choose an orthonormal basis.

Hence, it is useful to examine the effect of changing basis from one orthonormal basis to another. All the considerations of Section 2 apply, with the additional constraint that the matrix P is now a unitary matrix.** Namely, the transformation between any two orthonormal bases is always unitary. Suppose that the matrix A has the property that its eigenvectors comprise an orthonormal basis that spans the inner product space V. Following the discussion of Section 3, it follows that there exists a diagonalizing matrix U such that

$$U^\dagger A U = D\,,$$

where U is the unitary matrix ($U^\dagger = U^{-1}$) whose columns are the orthonormal eigenvectors of A and D is the diagonal matrix whose diagonal elements are the eigenvalues of A.

A *normal* matrix A is defined to be a matrix that commutes with its hermitian conjugate. That is,

$$A \text{ is normal} \qquad \Longleftrightarrow \qquad AA^\dagger = A^\dagger A\,.$$

In this section, we prove the matrix A can be diagonalized by a unitary similarity transformation if and only if it is normal.

We first prove that if A can be diagonalizable by a unitary similarity transformation, then A is normal. If $U^\dagger A U = D$, where D is a diagonal matrix, then $A = UDU^\dagger$ (using the fact that U is unitary). Then, $A^\dagger = UD^\dagger U^\dagger$ and

$$AA^\dagger = (UDU^\dagger)(UD^\dagger U^\dagger) = UDD^\dagger U^\dagger = UD^\dagger D U^\dagger = (UD^\dagger U^\dagger)(UDU^\dagger) = A^\dagger A\,.$$

In this proof, we use the fact that diagonal matrices commute with each other, so that $DD^\dagger = D^\dagger D$.

Conversely, if A is normal then it can be diagonalizable by a unitary similarity transformation. To prove this, consider the eigenvalue problem $A\vec{\boldsymbol{v}} = \lambda\vec{\boldsymbol{v}}$, where $\vec{\boldsymbol{v}} \neq 0$. All matrices possess at least one eigenvector and corresponding eigenvalue. Thus, we we focus on one of the eigenvalues and eigenvectors of A that satisfies $A\vec{\boldsymbol{v}}_1 = \lambda\vec{\boldsymbol{v}}_1$. We can always normalize $\vec{\boldsymbol{v}}_1$ to unity by dividing out by its norm. We now construct a unitary matrix U_1 as follows. Take the first column of U_1 to be given by (the normalized) $\vec{\boldsymbol{v}}_1$. The rest of the unitary matrix will be called Y, which is an $n \times (n-1)$ matrix. Explicitly,

$$U_1 = \left(\begin{array}{c:c} \vec{\boldsymbol{v}}_1 & Y \end{array} \right),$$

**In a real inner product space, a unitary transformation is real and hence is an orthogonal transformation.

where the vertical dashed line is inserted for the reader's convenience as a reminder that this is a *partitioned* matrix that is $n \times 1$ to the left of the dashed line and $n \times (n-1)$ to the right of the dashed line. Since the columns of U_1 comprise an orthonormal set of vectors, the matrix elements of Y are of the form

$$Y_{ij} = (\vec{\boldsymbol{v}}_j)_i\,, \qquad\qquad \text{for } i = 1, 2, \ldots, n \text{ and } j = 2, 3, \ldots,$$

where $\{\vec{\boldsymbol{v}}_1, \vec{\boldsymbol{v}}_2, \ldots, \vec{\boldsymbol{v}}_n\}$ is an orthonormal set of vectors. Here $(\vec{\boldsymbol{v}}_j)_i$ is the ith coordinate (with respect to a fixed orthonormal basis) of the jth vector of the orthonormal set. It then follows that the inner product of $\vec{\boldsymbol{v}}_j$ and $\vec{\boldsymbol{v}}_1$ is zero for $j = 2, 3, \ldots, n$. That is,

$$\langle \vec{\boldsymbol{v}}_j | \vec{\boldsymbol{v}}_1 \rangle = \sum_{k=1}^{n} (\vec{\boldsymbol{v}}_j)^*_k (\vec{\boldsymbol{v}}_1)_k = 0\,, \qquad \text{for} \qquad j = 2\,,\, 3\,,\, \ldots\,,\, n\,, \tag{19}$$

where $(\vec{\boldsymbol{v}}_j)^*_k$ is the complex conjugate of the kth component of the vector $\vec{\boldsymbol{v}}_j$. We can rewrite eq. (19) as a matrix product (where $\vec{\boldsymbol{v}}_1$ is an $n \times 1$ matrix) as:

$$Y^\dagger \vec{\boldsymbol{v}}_1 = \sum_{k=1}^{n} (Y)^*_{kj} (\vec{\boldsymbol{v}}_1)_k = \sum_{k=1}^{n} (\vec{\boldsymbol{v}}_j)^*_k (\vec{\boldsymbol{v}}_1)_k = 0\,. \tag{20}$$

We now compute the following product of matrices:

$$U_1^\dagger A U_1 = \left(\begin{array}{c} \vec{\boldsymbol{v}}_1^\dagger \\ \hdashline Y^\dagger \end{array}\right) A \left(\vec{\boldsymbol{v}}_1 \,\vdots\, Y \right) = \left(\begin{array}{c:c} \vec{\boldsymbol{v}}_1^\dagger A \vec{\boldsymbol{v}}_1 & \vec{\boldsymbol{v}}_1^\dagger A Y \\ \hdashline Y^\dagger A \vec{\boldsymbol{v}}_1 & Y^\dagger A Y \end{array}\right). \tag{21}$$

Note that the partitioned matrix above has the following structure:

$$\left(\begin{array}{c:c} 1 \times 1 & 1 \times (n-1) \\ \hdashline (n-1) \times 1 & (n-1) \times (n-1) \end{array}\right),$$

where we have indicated the dimensions (number of rows $\times$ number of columns) of the matrices occupying the four possible positions of the partitioned matrix. In particular, there is one row above the horizontal dashed line and $(n-1)$ rows below; there is one column to the left of the vertical dashed line and $(n-1)$ columns to the right. Using $A\vec{\boldsymbol{v}}_1 = \lambda_1 \vec{\boldsymbol{v}}_1$, with $\vec{\boldsymbol{v}}_1$ normalized to unity (*i.e.*, $\vec{\boldsymbol{v}}_1^\dagger \vec{\boldsymbol{v}}_1 = 1$), we see that:

$$\vec{\boldsymbol{v}}_1^\dagger A \vec{\boldsymbol{v}}_1 = \lambda_1 \vec{\boldsymbol{v}}_1^\dagger \vec{\boldsymbol{v}}_1 = \lambda_1\,,$$

$$Y^\dagger A \vec{\boldsymbol{v}}_1 = \lambda_1 Y^\dagger \vec{\boldsymbol{v}}_1 = 0\,.$$

after making use of eq. (20). Using these result in eq. (21) yields:

$$U_1^\dagger A U_1 = \left(\begin{array}{c:c} \lambda_1 & \vec{\boldsymbol{v}}_1^\dagger A Y \\ \hdashline 0 & Y^\dagger A Y \end{array}\right). \tag{22}$$

If A is normal then $U_1^\dagger A U_1$ is normal, since

$$\begin{aligned}
U_1^\dagger A U_1 (U_1^\dagger A U_1)^\dagger &= U_1^\dagger A U_1 U_1^\dagger A^\dagger U_1 = U_1^\dagger A A^\dagger U_1 \,, \\
(U_1^\dagger A U_1)^\dagger U_1^\dagger A U_1 &= U_1^\dagger A^\dagger U_1 U_1^\dagger A U_1 = U_1^\dagger A^\dagger A U_1 \,,
\end{aligned}$$

where we have used the fact that U_1 is unitary ($U_1 U_1^\dagger = \mathbf{I}$). Imposing $AA^\dagger = A^\dagger A$, we conclude that

$$U_1^\dagger A U_1 (U_1^\dagger A U_1)^\dagger = (U_1^\dagger A U_1)^\dagger U_1^\dagger A U_1 \,. \tag{23}$$

However, eq. (22) implies that

$$U_1^\dagger A U_1 (U_1^\dagger A U_1)^\dagger = \left(\begin{array}{c|c} \lambda_1 & \vec{\boldsymbol{v}}_1^\dagger A Y \\ \hline 0 & Y^\dagger A Y \end{array}\right) \left(\begin{array}{c|c} \lambda_1^* & 0 \\ \hline Y^\dagger A^\dagger \vec{\boldsymbol{v}}_1 & Y^\dagger A^\dagger Y \end{array}\right) = \left(\begin{array}{c|c} |\lambda_1|^2 + \vec{\boldsymbol{v}}_1^\dagger A Y Y^\dagger A^\dagger \vec{\boldsymbol{v}}_1 & \vec{\boldsymbol{v}}_1^\dagger A Y Y^\dagger A^\dagger Y \\ \hline Y^\dagger A Y Y^\dagger A^\dagger \vec{\boldsymbol{v}}_1 & Y^\dagger A Y Y^\dagger A^\dagger Y \end{array}\right) ,$$

$$(U_1^\dagger A U_1)^\dagger U_1^\dagger A U_1 = \left(\begin{array}{c|c} \lambda_1^* & 0 \\ \hline Y^\dagger A^\dagger \vec{\boldsymbol{v}}_1 & Y^\dagger A^\dagger Y \end{array}\right) \left(\begin{array}{c|c} \lambda_1 & \vec{\boldsymbol{v}}_1^\dagger A Y \\ \hline 0 & Y^\dagger A Y \end{array}\right) = \left(\begin{array}{c|c} |\lambda_1|^2 & \lambda_1^* \vec{\boldsymbol{v}}_1^\dagger A Y \\ \hline \lambda_1 Y^\dagger A^\dagger \vec{\boldsymbol{v}}_1 & Y^\dagger A^\dagger \vec{\boldsymbol{v}}_1 \vec{\boldsymbol{v}}_1^\dagger A Y + Y^\dagger A^\dagger Y Y^\dagger A Y \end{array}\right) .$$

Imposing the result of eq. (23), we first compare the upper left hand block of the two matrices above. We conclude that:

$$\vec{\boldsymbol{v}}_1^\dagger A Y Y^\dagger A^\dagger \vec{\boldsymbol{v}}_1 = 0 \,. \tag{24}$$

But $Y^\dagger A^\dagger \vec{\boldsymbol{v}}_1$ is an $(n-1)$-dimensional vector, so that eq. (24) is the matrix version of the following equation:

$$\langle Y^\dagger A^\dagger \vec{\boldsymbol{v}}_1 | Y^\dagger A^\dagger \vec{\boldsymbol{v}}_1 \rangle = 0 \,. \tag{25}$$

Since $\langle \vec{\boldsymbol{w}} | \vec{\boldsymbol{w}} \rangle = 0$ implies that $\vec{\boldsymbol{w}} = 0$ (and $\vec{\boldsymbol{w}}^\dagger = 0$), we conclude from eq. (25) that

$$Y^\dagger A^\dagger \vec{\boldsymbol{v}}_1 = \vec{\boldsymbol{v}}_1^\dagger A Y = 0 \,. \tag{26}$$

Using eq. (26) in the expressions for $U_1^\dagger A U_1 (U_1^\dagger A U_1)^\dagger$ and $(U_1^\dagger A U_1)^\dagger U_1^\dagger A U_1$ above, we see that eq. (23) requires that eq. (26) and the following condition are both satisfied:

$$Y^\dagger A Y Y^\dagger A^\dagger Y = Y^\dagger A^\dagger Y Y^\dagger A Y \,.$$

The latter condition simply states that $Y^\dagger A Y$ is normal. Using eq. (26) in eq. (22) then yields:

$$U_1^\dagger A U_1 = \left(\begin{array}{c|c} \lambda_1 & 0 \\ \hline 0 & Y^\dagger A Y \end{array}\right) , \tag{27}$$

where $Y^\dagger AY$ is normal. Thus, we have succeeded in reducing the original $n \times n$ normal matrix A down to an $(n-1)\times(n-1)$ normal matrix $Y^\dagger AY$, and we can now repeat the procedure again. The end result is the unitary diagonalization of A,

$$U^\dagger AU = D \equiv \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix} .$$

Moreover, the eigenvalues of A (which are complex in general) are the diagonal elements of D and the eigenvectors of A are the columns of U. This should be clear from the equation $AU = UD$. The proof given above does not care whether any degeneracies exist among the λ_i. Thus, we have proven that a normal matrix is diagonalizable by a unitary similarity transformation.

Since hermitian matrices and unitary matrices are normal, it immediately follows that hermitian and unitary matrices are also diagonalizable by a unitary similarity transformation. In the case of hermitian matrices, the corresponding eigenvalues λ_i must be real. In the case of unitary matrices, the corresponding eigenvalues are pure phases (i.e. complex numbers of unit magnitude).

Appendix: Proof that the eigenvectors corresponding to distinct eigenvalues are linearly independent

In this appendix, we shall prove that if $\vec{\boldsymbol{v}}_1, \vec{\boldsymbol{v}}_2, \ldots, \vec{\boldsymbol{v}}_n$ are eigenvectors corresponding to the distinct eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of A, then $\vec{\boldsymbol{v}}_1, \vec{\boldsymbol{v}}_2, \ldots, \vec{\boldsymbol{v}}_n$ are linearly independent. Recall that if $\vec{\boldsymbol{v}}_1, \vec{\boldsymbol{v}}_2, \ldots, \vec{\boldsymbol{v}}_n$ are linearly independent, then

$$c_1\vec{\boldsymbol{v}}_1 + c_2\vec{\boldsymbol{v}}_2 + \cdots + c_n\vec{\boldsymbol{v}}_n = 0 \qquad \Longleftrightarrow \qquad c_i = 0 \text{ for all } i = 1, 2, \ldots, n\,. \tag{28}$$

Starting from $A\vec{\boldsymbol{v}} = \lambda\vec{\boldsymbol{v}}$, we multiply on the left by A to get

$$A^2\vec{\boldsymbol{v}} = A\cdot A\vec{\boldsymbol{v}} = A(\lambda\vec{\boldsymbol{v}}) = \lambda A\vec{\boldsymbol{v}} = \lambda^2\vec{\boldsymbol{v}}\,.$$

Continuing this process of multiplication on the left by A, we conclude that:

$$A^k\vec{\boldsymbol{v}} = A\left(A^{k-1}\vec{\boldsymbol{v}}\right) = A\left(\lambda^{k-1}\vec{\boldsymbol{v}}\right) = \lambda^{k-1}A\vec{\boldsymbol{v}} = \lambda^k\vec{\boldsymbol{v}}\,, \tag{29}$$

for $k = 2, 3, \ldots, n$. Thus, if we multiply eq. (28) on the left by A^k, then we obtain n separate equations by choosing $k = 0, 1, 2, \ldots, n-1$ given by:

$$c_1\lambda_1^k\vec{\boldsymbol{v}}_1 + c_2\lambda_2^k\vec{\boldsymbol{v}}_2 + \cdots + c_n\lambda_n^k\vec{\boldsymbol{v}}_n = 0\,, \qquad k = 0, 1, 2, \ldots, n-1\,.$$

In matrix form,

$$\begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ \lambda_1 & \lambda_2 & \lambda_3 & \cdots & \lambda_n \\ \lambda_1^2 & \lambda_2^2 & \lambda_3^2 & \cdots & \lambda_n^2 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \lambda_1^{n-1} & \lambda_2^{n-1} & \lambda_3^{n-1} & \cdots & \lambda_n^{n-1} \end{pmatrix} \begin{pmatrix} c_1\vec{\boldsymbol{v}}_1 \\ c_2\vec{\boldsymbol{v}}_2 \\ c_3\vec{\boldsymbol{v}}_3 \\ \vdots \\ c_n\vec{\boldsymbol{v}}_n \end{pmatrix} = 0\,. \tag{30}$$

The matrix appearing above is equal to the transpose of a well known matrix called the Vandermonde matrix. There is a beautiful formula for its determinant:

$$\begin{vmatrix} 1 & 1 & 1 & \cdots & 1 \\ \lambda_1 & \lambda_2 & \lambda_3 & \cdots & \lambda_n \\ \lambda_1^2 & \lambda_2^2 & \lambda_3^2 & \cdots & \lambda_n^2 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \lambda_1^{n-1} & \lambda_2^{n-1} & \lambda_3^{n-1} & \cdots & \lambda_n^{n-1} \end{vmatrix} = \prod_{i<j} (\lambda_i - \lambda_j)\,. \tag{31}$$

I leave it as a challenge to the reader for providing a proof of eq. (31). This result implies that if all the eigenvalues λ_i are distinct, then the determinant of the Vandermonde matrix is nonzero. In this case, the Vandermonde matrix is invertible. Multiplying eq. (30) by the inverse of the Vandermonde matrix then yields $c_i \vec{\boldsymbol{v}}_i = 0$ (no sum over i) for all $i = 1, 2, \ldots, n$. Since the eigenvectors are nonzero by definition, it follows that $c_i = 0$ for all $i = 1, 2, \ldots, n$. Hence the $\{\vec{\boldsymbol{v}}_i\}$ are linearly independent.