Linear Operators / Functions as Vectors

Overview and Motivation: We first introduce the concept of linear operators on a vector space. We then look at some more vector-space examples, including a space where the vectors are functions.

Key Mathematics: More vector-space math!

I. Linear Operators

A. Definition and Examples

The essential nature of a **linear operator** is contained in its name. The operator part of the name means that a linear operator A operates on any vector $\mathbf{u}$ (in the space of interest) and produces another vector $\mathbf{v}$ in the space. That is, if $\mathbf{u}$ is a vector, then

$$\mathbf{v} = A\mathbf{u} \tag{1}$$

is also vector. The linear part of linear operator means that

$$A(a\,\mathbf{u} + b\,\mathbf{v}) = a\,A\mathbf{u} + b\,A\mathbf{v} \tag{2}$$

is satisfied for all scalars a and b and all vectors $\mathbf{u}$ and $\mathbf{v}$ in the space.

Linear operators come in many different forms. The ones of interest for any given vector space depend upon the problem being solved. When dealing with a vector space of finite dimension, we can always use standard linear-algebra notation to represent the vectors as **column matrices** of length N and the linear operators as **square matrices** of size $N \times N$. For $N = 3$, for example, Eq. (1) can be written as

$$\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix}, \tag{3}$$

where v_i, u_i, and A_{ij} are the (scalar) components of $\mathbf{v}$, $\mathbf{u}$, and A, respectively, in some particular orthonormal basis.[1]

As we shall see below, sometimes we are interested in a vector space where the vectors are functions. In that case the linear operators of interest may be linear

[1] For example, if dealing with vectors in real space, the elements in a column vector are often the scalar components (also known as Cartesian coordinates) of that vector in the $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, $\hat{\mathbf{z}}$ basis.

differential operators. An example of a **linear differential operator** on a vector space of functions of x is d/dx. In this case Eq. (1) looks like

$$g(x) = \frac{d}{dx} f(x), \tag{4}$$

where $f(x)$ and $g(x)$ are vectors in the space and d/dx is the linear operator.

B. Eigenvalue Problems

An important vector-space problem is the eigenvalue problem. We already have some experience with this problem as part of the process of finding the normal modes of the coupled oscillators. Simply stated, the **eigenvalue problem** is this: for a given linear operator A, what are the vectors $\mathbf{u}$ and scalars λ such that

$$A\mathbf{u} = \lambda\mathbf{u} \tag{5}$$

is satisfied? These vectors $\mathbf{u}$ and scalars λ are obviously special to the operator: when operated on by A, these vectors only change by the scale factor λ. These special vectors $\mathbf{u}$ are known as **eigenvectors** and the values of λ are known as **eigenvalues**. Each eigenvector $\mathbf{u}$ has associated with it a particular eigenvalue λ.

For a vector space of N dimensions (where we are using standard linear algebra notation) the eigenvalues are solutions of the **characteristic equation**

$$\det(A - \lambda I) = 0, \tag{8}$$

where I is the **identity matrix**. As we did when solving the $N = 2$ and $N = 3$ (homework) coupled oscillator problems, substituting the eigenvalues (one at a time!) back into Eq. (5) allows us to find the eigenvectors $\mathbf{u}$.

If the (finite dimension) vector space is complex then Eq. (8) always has solutions.[2] Now here is the cool thing. If the operator is **self-adjoint** (also know as **Hermitian**), which means that its matrix elements satisfy $A_{ji} = A_{ij}^*$, then

(*i*) its eigenvalues are real,
(*ii*) its eigenvectors span the space, and
(*iii*) the eigenvectors with distinct eigenvalues are orthogonal.

Thus, if the operator A is self-adjoint and all eigenvalues are distinct, then those eigenvectors form an orthogonal basis for the space. If the eigenvalues are not

[2] This result is known as the fundamental theorem of algebra.

distinct, an orthogonal basis can still be formed from the eigenvectors. (it just takes a little bit of work.)

Often, however, the eigenvalue problem of interest is on a real vector space. In this case, if A is **symmetric** (that is, the matrix elements of A satisfy $A_{ij} = A_{ji}$), then Eq. (8) will have N real solutions and, again, the associated eigenvectors $\mathbf{u}$ can be used to form a basis for the vector space.

A famous eigenvalue problem from quantum mechanics is none other than the time-independent **Schrödinger equation**

$$H\psi = E\psi , \tag{6}$$

which is an eigenvalue problem on a vector space of functions. Here the vectors are the functions $\psi(x, y, z)$; the operator is the differential operator

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(x, y, z); \tag{7}$$

and the eigenvalues are specific values of E.[3] This is perhaps the most important equation in quantum mechanics because the (normalized) eigenvectors describe the (spatial part of the) states of the system with a definite value of energy, and the eigenvalues E are the energies of those states.

II. The Coupled Oscillator Problem Redux

Let's revisit the coupled oscillator problem to see how that problem fits into our discussion of vector spaces. We first review the associated eigenvalue problem that we solved when finding the normal modes, and then we make some remarks about the initial-value problem.

A. The Eigenvalue Problem

Recall, in that problem we started with N equations of motion (one for each object)

$$\ddot{q}_j - \tilde{\omega}^2\left(q_{j-1} - 2q_j + q_{j+1}\right) = 0 , \tag{9}$$

($j = 1, \ldots, N$), where $q_j(t)$ is the time-dependent displacement of the jth oscillator. We then looked for normal-mode solutions

[3] The function $V(x, y, z)$ is the classical potential energy a particle of mass m.

$$q_j(t) = q_{0,j} e^{i\Omega t}, \tag{10}$$

where all N objects oscillate at the same frequency Ω. By assuming that the solutions had the form of Eq. (10), the N coupled ordinary differential equations became the N coupled algebraic equations

$$\Omega^2 q_{0,j} + \tilde{\omega}^2 \left(q_{0,j-1} - 2q_{0,j} + q_{0,j+1} \right) = 0, \tag{11}$$

which we rewrote as

$$\begin{pmatrix} 2\tilde{\omega}^2 & -\tilde{\omega}^2 & 0 & 0 & \\ -\tilde{\omega}^2 & 2\tilde{\omega}^2 & -\tilde{\omega}^2 & 0 & \\ 0 & -\tilde{\omega}^2 & 2\tilde{\omega}^2 & -\tilde{\omega}^2 & \cdots \\ 0 & 0 & -\tilde{\omega}^2 & 2\tilde{\omega}^2 & \\ & & \vdots & & \end{pmatrix} \begin{pmatrix} q_{0,1} \\ q_{0,2} \\ q_{0,3} \\ \vdots \\ q_{0,N} \end{pmatrix} = \Omega^2 \begin{pmatrix} q_{0,1} \\ q_{0,2} \\ q_{0,3} \\ \vdots \\ q_{0,N} \end{pmatrix} \tag{12}$$

Notice that this is exactly of the form of Eq. (5) (the eigenvalue problem) where the vectors are $N-$row column matrices, the linear operator A is an $N \times N$ matrix, and the eigenvalues λ are the squared frequencies Ω^2.

As we previously discovered in solving that problem there are N eigenvectors,

$$\begin{pmatrix} q_{0,1} \\ q_{0,2} \\ q_{0,3} \\ \vdots \\ q_{0,N} \end{pmatrix}_n = \begin{pmatrix} \sin\left(\frac{n\pi}{N+1} 1\right) \\ \sin\left(\frac{n\pi}{N+1} 2\right) \\ \sin\left(\frac{n\pi}{N+1} 3\right) \\ \vdots \\ \sin\left(\frac{n\pi}{N+1} N\right) \end{pmatrix} \tag{13}$$

($n = 1, \ldots, N$), and the nth eigenvector has the eigenvalue

$$\Omega_n^2 = 4\tilde{\omega}^2 \sin^2\left(\frac{n\pi}{2(N+1)} \right). \tag{14}$$

Notice that the eigenvalues are real, as they should be for a symmetric operator. Also, because the eigenvalues are distinct, the eigenvectors from an orthogonal basis for the space.

B. The Initial Value Problem

As part of solving the initial-value problem for this system, we ended up with the equation[4]

$$\begin{pmatrix} q_1(0) \\ q_2(0) \\ q_3(0) \\ \vdots \\ q_N(0) \end{pmatrix} = \sum_{n=1}^{N} \mathrm{Re}(a_n) \begin{pmatrix} \sin\left(\frac{n\pi}{N+1}1\right) \\ \sin\left(\frac{n\pi}{N+1}2\right) \\ \sin\left(\frac{n\pi}{N+1}3\right) \\ \vdots \\ \sin\left(\frac{n\pi}{N+1}N\right) \end{pmatrix}, \tag{15}$$

which we needed to solve for the coefficients $\mathrm{Re}(a_n)$. Let's now place the previous solution of Eq. (15) for the coefficients $\mathrm{Re}(a_n)$ within the context of the current discussion of vector spaces.[5] As we talked about in the last lecture, if we write a vector $\mathbf{v}$ as a linear combination of orthogonal vectors $\mathbf{u}_n$

$$\mathbf{v} = \sum_{n=1}^{N} v_n \mathbf{u}_n , \tag{16}$$

then the coefficients v_n in are given by

$$v_n = \frac{(\mathbf{u}_n, \mathbf{v})}{(\mathbf{u}_n, \mathbf{u}_n)} . \tag{17}$$

For the example at hand, Eq. (15) is equivalent to Eq. (16), but in order apply Eq. (17) to find the coefficients $\mathrm{Re}(a_n)$ in Eq. (15), we need the definition of the inner product of two vectors for this vector space. For any N dimensional vector space the inner product between two vectors $\mathbf{w}$ and $\mathbf{v}$ can be written as (See Exercise 14.5)

$$(\mathbf{w}, \mathbf{v}) = \begin{pmatrix} w_1^* & w_2^* & \ldots & w_N^* \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{pmatrix}, \tag{18}$$

where w_n and v_n are the components of the vectors $\mathbf{w}$ and $\mathbf{v}$ in the same basis. Notice that the elements of the row matrix in Eq. (18) are the complex conjugates of

[4] This is Eq. (10) of the Lecture 10 notes.

[5] Note that Eq. (15) says, at its most basic level, that the eigenvectors [Eq. (13)] form a basis for the space of initial displacements of the objects (which can be any set of N real numbers).

the elements of $\mathbf{u}$. Of course, if we are dealing with real vector, then the complex conjugate is simply the element itself. Note that Eq. (18) can be written in more compact form as

$$(\mathbf{w},\mathbf{v}) = \sum_{j=1}^{N} w_j^* v_j \ . \tag{19}$$

Using the form of the inner product in Eq. (19), the application of Eq. (17) to the coupled oscillator problem is thus[6]

$$\mathrm{Re}(a_n) = \frac{\sum_{j=1}^{N} \sin\left(\frac{n\pi}{N+1} j\right) q_j(0)}{\sum_{j=1}^{N} \sin^2\left(\frac{n\pi}{N+1} j\right)} . \tag{20}$$

III. Vectors Spaces and Fourier Series

The last vector-space example is Fourier Series. Recall, the complex Fourier-series representation of a function $f(x)$ defined on the interval $-L$ to L is

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{in\pi x/L} , \tag{21a}$$

where the coefficients c_n are given by

$$c_n = \frac{1}{2L} \int_{-L}^{L} f(x)\, e^{-in\pi x/L}\, dx . \tag{21b}$$

If you have been paying attention to this point (i.e, if you are still awake), then you should be thinking "Ah ha! Equation (21) says that we can write the function $f(x)$ as a linear combination of the (basis!) functions $e^{in\pi x/L}$ with coefficients c_n. Looks like a vector space to me! And ah ha, again! It seems that somehow Eq. (21b) is the equivalent of Eq. (17), where the coefficients are expressed in terms of inner products on this space." But likely you are now asleep and thinking about other things.

But if you were awake, you would be entirely correct. Let's see that this is the case. The vectors in this space are indeed functions on the interval $-L$ to L, and one set of

[6] Equation (20) is Eq. (18) of the Lecture 10 notes.

basis vectors $\mathbf{u}_n$ is indeed the set of functions $u_n(x) = e^{in\pi x/L}$, $-\infty < n < \infty$. So what is the inner product on this space that makes these basis vectors orthogonal? You actually saw the inner product back in Lecture 12 before you knew it was an inner product, so let me remind you. Denoting, for example, a function $f(x)$ as the vector $\mathbf{f}$, we define the inner product $(\mathbf{g},\mathbf{f})$ in this space as

$$(\mathbf{g},\mathbf{f}) = \int_{-L}^{L} g^*(x) f(x) dx . \tag{22}$$

Again, note the complex conjugate in the definition. Also notice the similarity of Eqs. (19) and (22). Using Eq. (22), Eq. (21) can be written in vector-space notation as

$$\mathbf{f} = \sum_{n=-\infty}^{\infty} c_n \mathbf{u}_n , \tag{23a}$$

$$c_n = \frac{(\mathbf{u}_n,\mathbf{f})}{(\mathbf{u}_n,\mathbf{u}_n)} . \tag{23b}$$

Lastly, let's revisit the idea of an orthonormal basis within the context of Fourier series. Recall, a normalized (or unit) vector $\hat{\mathbf{u}}$ is defined by $\|\hat{\mathbf{u}}\| = \sqrt{(\hat{\mathbf{u}},\hat{\mathbf{u}})} = 1$, and we can normalize any vector $\mathbf{u}$ via

$$\hat{\mathbf{u}} = \frac{\mathbf{u}}{\sqrt{(\mathbf{u},\mathbf{u})}} . \tag{25}$$

Let's find the normalized version of the basis functions $u_n(x) = e^{in\pi x/L}$. Calculating $(\mathbf{u}_n,\mathbf{u}_n)$ we have

$$(\mathbf{u}_n,\mathbf{u}_n) = \int_{-L}^{L} e^{-in\pi x/L} e^{in\pi x/L} dx = 2L . \tag{26}$$

We can thus turn our *orthogonal* basis into an *orthonormal* basis by using the normalized vectors

$$\hat{\mathbf{u}}_n = \frac{e^{in\pi x/L}}{\sqrt{2L}} . \tag{27}$$

If we now write a vector in this space as a linear combination of these normalized basis vectors,

$$\mathbf{f} = \sum_{n=-\infty}^{\infty} c_n \hat{\mathbf{u}}_n \ , \tag{28a}$$

$$c_n = \left(\hat{\mathbf{u}}_n, \mathbf{f}\right) \tag{28b}$$

then the functional expression of Eq. (28) results in the Fourier series being written as

$$f(x) = \frac{1}{\sqrt{2L}} \sum_{n=-\infty}^{\infty} c_n e^{in\pi x/L} \ , \tag{29a}$$

$$c_n = \frac{1}{\sqrt{2L}} \int_{-L}^{L} f(x) e^{-in\pi x/L}\, dx \ . \tag{29b}$$

To some, the Fourier Series written as Eq. (29) is more appealing because it has a certain symmetry that Eq. (21) lacks.

Exercises

***14.1** Consider the operator $A = \begin{pmatrix} i & j \\ k & l \end{pmatrix}$ on a two dimensional vector space. Show that for any two scalars a and b and any two vectors $\mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$ and $\mathbf{v} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$ that this operator is linear, i.e., that it satisfies Eq. (2).

***14.2** Show that for any two scalars a and b and any two functions $f(x)$ and $g(x)$, that the differential operator $i\frac{d}{dx}$ is linear, i.e., that it satisfies Eq. (2).

***14.3** In solving the $N = 3$ coupled oscillator problem, we found the three eigenvectors to the associated eigenvalue problem, which can be written as

$\mathbf{u}_1 = \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}$, $\mathbf{u}_2 = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$, and $\mathbf{u}_1 = \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}$. Find the normalized versions $\hat{\mathbf{u}}_1$, $\hat{\mathbf{u}}_2$, and $\hat{\mathbf{u}}_3$ of each of these vectors.

****14.4** Consider the time independent Schrödinger equation eigenvalue problem $H\psi = E\psi$, where H is the operator $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}kx^2$. This is the (1D) quantum mechanical harmonic-oscillator problem. The solutions (eigenvectors and eigenvalues) of this problem can be written as $(n = 0,1,2,\ldots)$

$$\psi_n(x) = \left(\frac{d}{dx} - ax\right)^n e^{-ax^2/2}, \text{ where } a = \sqrt{mk/\hbar^2} \text{ and}$$

$$E_n = \frac{\hbar\tilde{\omega}}{2} + n\hbar\tilde{\omega}, \text{ where } \tilde{\omega} = \sqrt{k/m}$$

(**a**) For $n = 0$ (the ground state), show that $\psi_0(x)$ is a solution to $H\psi = E\psi$ with the appropriate eigenvalue.
(**b**) For this vector space, the inner product of two vectors $\boldsymbol{\psi}$ and $\boldsymbol{\varphi}$ is defined as $(\boldsymbol{\varphi}, \boldsymbol{\psi}) = \int_{-\infty}^{\infty} \varphi^*(x)\psi(x)dx$. Show that the $n = 0$ and $n = 1$ states are orthogonal.
(**c**) Find the norm of the $n = 0$ state. Thus construct the normalized eigenvector corresponding to this state.
(**d**) Given that $H\psi_0 = E_0\psi_0$ and $H\psi_1 = E_1\psi_1$, find $H\varphi$, where $\varphi = C_0\psi_0 + C_1\psi_1$ (Here $C_0 \neq 0$ and $C_1 \neq 0$ are two constants.) Thus argue that the wave function φ is *not* an eigenvector of H (for any value of E).

***14.5 Inner product**. Consider two vectors written in terms of some orthonormal basis,

$$\mathbf{v} = \sum_{n=1}^{N} v_n \mathbf{u}_n, \ \mathbf{w} = \sum_{m=1}^{N} w_m \mathbf{u}_m .$$

(**a**) Using Eq. (10) of the Lecture 13 notes, show that the inner product $(\mathbf{w}, \mathbf{v})$ can be expressed in terms of the components of the two vectors as $(\mathbf{w}, \mathbf{v}) = \sum_{n=1}^{N} w_n^* v_n$.
(**b**) What is the norm of the vector $\mathbf{v}$ expressed in terms of its components?

*__14.6 Inner Product and Fourier Series__. Consider two functions expressed as their normalized Fourier Series representations,

$$f(x)=\frac{1}{\sqrt{2L}}\sum_{n=-\infty}^{\infty}c_n e^{in\pi x/L}\ ,\ g(x)=\frac{1}{\sqrt{2L}}\sum_{m=-\infty}^{\infty}d_n e^{im\pi x/L}\ .$$

(**a**) Starting with these expressions, show that the inner product $(\mathbf{g},\mathbf{f})=\int_{-L}^{L} g^*(x)f(x)dx$ can be expressed in terms of the Fourier coefficients c_n and d_n as $(\mathbf{g},\mathbf{f})=\sum_{n=-\infty}^{\infty} d_n^* c_n$.

(**b**) What is the norm of $f(x)$ in terms of its Fourier coefficients?

Notice the similarity of these results and those of Exercise 14.5. Cool, eh?