

Applications

- Spectral graph theory and consensus algorithms
- Gram and Covariance matrices
 - Spectral clustering
- Applications to image processing.

Topics

- Eigenvalues of Symmetric Matrices (ALA 8.5)
- Quadratic forms and positive definite matrices (ALA 3.4, LAA 7.2)
- Optimization Principles for Eigenvalues of Symmetric Matrices (ALA 8.5)

Eigenvalues of Symmetric Matrices

A square matrix A is said to be **symmetric** if $A=A^T$. For example, all 2×2 symmetric and 3×3 symmetric matrices are of the form:

$$\begin{bmatrix} a & b \\ b & c \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} a & b & c \\ b & d & e \\ c & e & f \end{bmatrix}.$$

Symmetric matrices arise in many practical contexts; an important one we will spend time on next class are **covariance matrices**. For now, we simply take them as a family of interesting matrices.

Symmetric matrices enjoy many interesting properties, including the following one which will be the focus, of this lecture:

Theorem: Let $A=A^T \in \mathbb{R}^{n \times n}$ be a symmetric $n \times n$ matrix. Then:

- (a) All eigenvalues of A are real.
- (b) Eigenvectors corresponding to distinct eigenvalues of A are orthogonal.
- (c) There is an orthonormal basis of \mathbb{R}^n consisting of n eigenvectors of A .

In particular, all real symmetric matrices are complete and real diagonalizable.

We'll spend the rest of this lecture exploring the consequences of this remarkable theorem, before diving into applications over the next few classes.

First, we work through a few simple examples to see this theorem in action.

Example: $A = \begin{bmatrix} 3 & 1 \\ 1 & 3 \end{bmatrix}$; We've seen this matrix in previous examples. It has

eigenvalues $\lambda_1 = 4$ and $\lambda_2 = 2$ with corresponding eigenvectors $\underline{v}_1 = (1, 1)$ and $\underline{v}_2 = (-1, 1)$. We easily verify that $\underline{v}_1^T \underline{v}_2 = 0$, and hence are orthogonal. We construct an orthonormal basis by dividing each eigenvector by its Euclidean norm:

$$\underline{u}_1 = \frac{\underline{v}_1}{\|\underline{v}_1\|} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad \text{and} \quad \underline{u}_2 = \frac{\underline{v}_2}{\|\underline{v}_2\|} = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 1 \end{bmatrix}.$$

Example: Consider the symmetric matrix $A = \begin{bmatrix} 5 & -4 & 2 \\ -4 & 5 & 2 \\ 2 & 2 & -1 \end{bmatrix}$. Computing

the eigenvalues/eigenvectors of A (e.g., using np.linalg.eigs) we see that $\lambda_1 = 9, \underline{v}_1 = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}$, $\lambda_2 = 3, \underline{v}_2 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$, and $\lambda_3 = -3, \underline{v}_3 = \begin{bmatrix} 1 \\ 1 \\ -2 \end{bmatrix}$.

You can check that these vectors are pairwise orthogonal: $\underline{v}_i^T \underline{v}_j = 0$ for $i \neq j$, and hence form an orthogonal basis for \mathbb{R}^3 . An orthonormal basis is obtained by the corresponding unit norm eigenvectors:

$$\underline{u}_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 1 \\ 0 \end{bmatrix}, \quad \underline{u}_2 = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, \quad \text{and} \quad \underline{u}_3 = \frac{1}{\sqrt{6}} \begin{bmatrix} 1 \\ 1 \\ -2 \end{bmatrix}.$$

The Spectral Theorem

The theorem above tells us that every real, symmetric matrix admits an eigenvector basis, and hence is diagonalizable. Furthermore, we can always choose eigenvectors that form an orthonormal basis — hence, the diagonalizing matrix takes a particularly simple form.

Remember that a matrix $Q \in \mathbb{R}^{n \times n}$ is orthogonal if and only if its columns form an orthonormal basis of \mathbb{R}^n . Alternatively, we can characterize orthogonal matrices by the condition that $Q^T Q = Q Q^T = I$, i.e., $Q^{-1} = Q^T$.

If we use this orthonormal eigenbasis when diagonalizing a symmetric matrix A , we obtain its spectral factorization.

Theorem: Let A be a real symmetric matrix. Then there exists an orthogonal matrix Q such that

$$A = Q \Lambda Q^{-1} = Q \Lambda Q^T \quad (\text{ST})$$

where Λ is a real diagonal matrix. The eigenvalues of A appear on the diagonal of Λ , while the columns of Q are the corresponding orthonormal eigenvectors.

Historical Remark: The term "spectrum" refers to the eigenvalues of a matrix, or more generally, a linear operator. This terminology originates in physics: the spectral energy lines of atoms, molecules, and nuclei are characterized as the eigenvalues of the governing quantum mechanical Schrödinger operator.

Example: For $A = \begin{bmatrix} 3 & 1 \\ 1 & 3 \end{bmatrix}$ seen above, we build $Q = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$, and write

$$\begin{bmatrix} 3 & 1 \\ 1 & 3 \end{bmatrix} = A = Q \Lambda Q^T = \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 4 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}.$$

Geometric Interpretation

You can always choose Q to have $\det Q = 1$; such a Q represents a rotation. Thus the diagonalization of a symmetric matrix can be interpreted as a rotation of the coordinate system so that the orthogonal eigenvectors align with the coordinate

axes. Therefore, the linear transformation $L(x) = Ax$ for which A has all positive eigenvalues can be interpreted as a combination of stretches in n mutually orthogonal directions. One way to visualize this is to consider what $L(x)$ does to the unit Euclidean sphere $S = \{x \in \mathbb{R}^n \mid \|x\| = 1\}$: stretching it in orthogonal directions will transform it into an ellipsoid: $E = L(S) = \{Ax \mid \|x\| = 1\}$ whose principal axes are the directions of stretch, i.e., the eigenvectors of A .

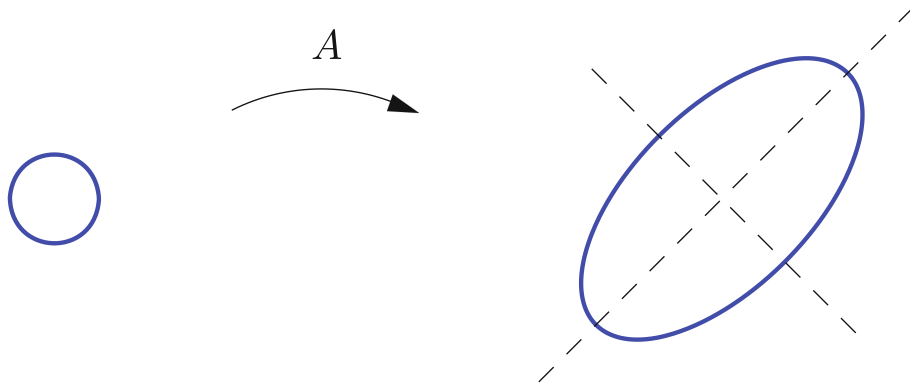


Figure 8.3. Stretching a Circle into an Ellipse.

Quadratic Forms & Positive Definite Matrices (ALA 3.4, LAA 7.2)

One common place where symmetric matrices arise in application is in defining **quadratic forms**, which pop up in engineering design (in design criteria and optimization), signal processing (as output noise power), physics (as potential & kinetic energy), differential geometry (as normal curvature of surfaces), economics (as utility functions), and statistics (in confidence ellipsoids).

A **quadratic form** is a function mapping \mathbb{R}^n to \mathbb{R} of the form

$$q(z) = z^T K z \quad (\text{QF})$$

where $K = K^T \in \mathbb{R}^{n \times n}$ is an $n \times n$ symmetric matrix. Such quadratic forms arise frequently in applications of linear algebra. For example, setting $K = I_n$ and $z = Ax - b$, we recover the least-squares objective

$$q(Ax - b) = (Ax - b)^T (Ax - b) = \|Ax - b\|^2$$

Example: For $\underline{x} \in \mathbb{R}^3$, let $q(\underline{x}) = 5x_1^2 + 3x_2^2 + 2x_3^2 - x_1x_2 + 6x_2x_3$. Find a matrix $k = k^T \in \mathbb{R}^{3 \times 3}$ such that $q(\underline{x}) = \underline{x}^T k \underline{x}$.

The approach is to recognize that the coefficients of x_1^2 , x_2^2 , and x_3^2 go on the diagonal of k . To make k symmetric, the coefficients for $x_i x_j$, $i \neq j$, should be evenly split between the (i,j) and (j,i) entries of k .

Using this strategy, we obtain:

$$q(\underline{x}) = \underline{x}^T k \underline{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}^T \begin{bmatrix} 5 & -1/2 & 0 \\ -1/2 & 3 & 4 \\ 0 & 4 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}.$$

The Geometry of Quadratic Forms

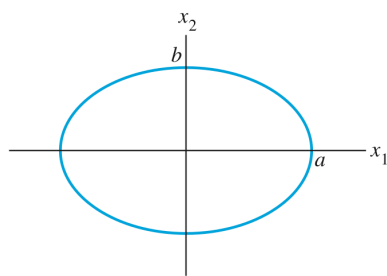
We'll focus on understanding the geometry of quadratic forms on $\mathbb{R}^{2 \times 2}$. Let $k = k^T \in \mathbb{R}^{2 \times 2}$ be an invertible 2×2 symmetric matrix, and let's consider quadratic forms:

$$q(\underline{x}) = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^T \begin{bmatrix} k_{11} & k_{12} \\ k_{12} & k_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = k_{11}x_1^2 + 2k_{12}x_1x_2 + k_{22}x_2^2 \quad (2D).$$

What kinds of functions do these define? We study this question by looking at the level sets of $q(\underline{x})$. The α -level set of $q(\underline{x})$ is the set of all $\underline{x} \in \mathbb{R}^2$ such that $q(\underline{x}) = \alpha$:

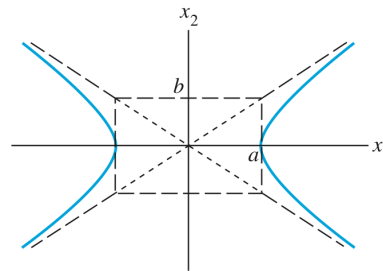
$$C_\alpha = \{ \underline{x} \in \mathbb{R}^2 : q(\underline{x}) = \alpha \}. \quad (\alpha)$$

It is possible to show that such level sets correspond to either an ellipse, a hyperbola, two intersecting lines, or no points at all. If k is a diagonal matrix, the graph of (α) is in standard position, as seen below:



$$\frac{x_1^2}{a^2} + \frac{x_2^2}{b^2} = 1, \quad a > b > 0$$

ellipse



$$\frac{x_1^2}{a^2} - \frac{x_2^2}{b^2} = 1, \quad a > b > 0$$

hyperbola

FIGURE 2 An ellipse and a hyperbola in standard position.

If k is not diagonal, the graph of (α) is rotated out of standard position, as shown below:

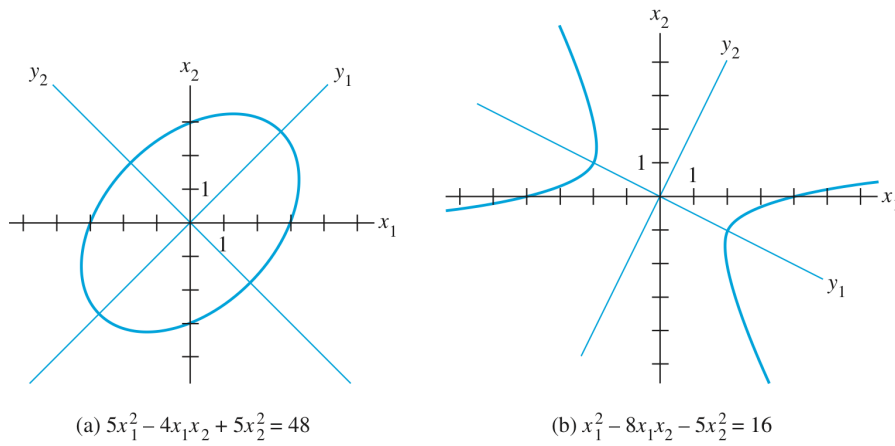


FIGURE 3 An ellipse and a hyperbola *not* in standard position.

The principle axes of these rotated graphs are defined by the eigenvectors of K , and amount to a new coordinate system (or change of basis) with respect to which the graph is in standard position.

Example: The ellipse in Fig. 3a is the graph of equation $5x_1^2 - 4x_1x_2 + 5x_2^2 = 48$. This is given by the quadratic form

$$q(\underline{x}) = \underline{x}^T K \underline{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^T \begin{bmatrix} 5 & -2 \\ -2 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}.$$

The eigenvalues/vectors of K are:

$$\lambda_1 = 3, \underline{v}_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad \text{and} \quad \lambda_2 = 7, \underline{v}_2 = \begin{bmatrix} -1 \\ 1 \end{bmatrix}.$$

We define the orthonormal basis: $\underline{u}_1 = \frac{\underline{v}_1}{\|\underline{v}_1\|} = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$ and $\underline{u}_2 = \frac{\underline{v}_2}{\|\underline{v}_2\|} = \begin{bmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$

and set $Q = [\underline{u}_1, \underline{u}_2] = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$. Then $q(\underline{x}) = \underline{x}^T Q \Lambda Q^T \underline{x}$, and the change of variables $\underline{y} = Q^T \underline{x}$ produces the quadratic form

$$q(\underline{y}) = \underline{y}^T \Lambda \underline{y} = 3y_1^2 + 7y_2^2.$$

These axes are shown in Fig. 3a (labeled y_1 and y_2).

Classifying Quadratic Forms

Depending on the eigenvalues of the symmetric matrix K defining a quadratic form $q(\underline{x}) = \underline{x}^T K \underline{x}$, the resulting function can look very different. The figure below shows four different quadratic forms plotted as functions with domain \mathbb{R}^2 , i.e., we are plotting $(x, y, q(x, y))$:

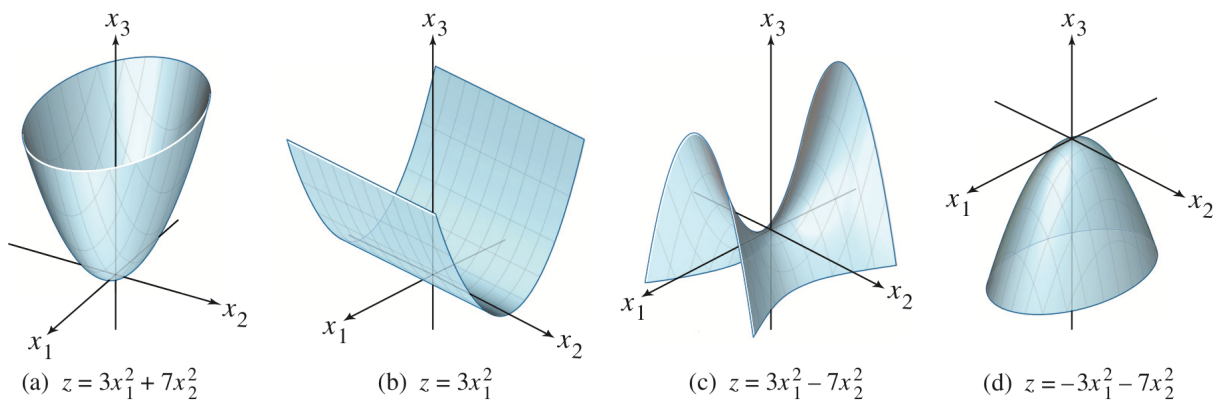


FIGURE 4 Graphs of quadratic forms.

Notice that except for $\underline{x} = \underline{0}$, the values $q(\underline{x})$ are all positive in Fig. 4(b) and all negative in Fig. 4(d). If we take horizontal cross-sections of these plots, we get an ellipse (these are the level sets C_α we saw earlier!); the horizontal cross-sections of 4(c) are hyperbolas.

This simple 2D example illustrates the following definitions. A quadratic form Q is:

- (a) positive definite if $q(\underline{x}) > 0$ for all $\underline{x} \neq \underline{0}$
- (b) negative definite if $q(\underline{x}) < 0$ for all $\underline{x} \neq \underline{0}$
- (c) indefinite if $q(\underline{x})$ assumes both positive and negative values.

Also, $q(\underline{x})$ is said to be positive (negative) semidefinite if $q(\underline{x}) \geq 0$ (≤ 0) all \underline{x} : in particular, we now allow $q(\underline{x}) = 0$ for nonzero \underline{x} .

The following theorem leverages the spectral factorization of a symmetric matrix to characterize quadratic forms in terms of the eigenvalues of K :

Theorem: Let $K = K^T \in \mathbb{R}^{n \times n}$ be a symmetric $n \times n$ matrix. Then a quadratic form is:

- (a) positive definite if and only if all eigenvalues of K are positive;
- (b) negative definite if and only if all eigenvalues of K are negative;
- (c) indefinite if and only if K has both positive and negative eigenvalues.

Proof: Let $K = Q \Lambda Q^T$ be the spectral factorization of K : Q has columns defining an orthonormal eigenbasis for \mathbb{R}^n and $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n)$ is a diagonal matrix of eigenvalues of K . Then:

$$\begin{aligned}
 q(\underline{x}) &= \underline{x}^T K \underline{x} = \underline{x}^T Q \Lambda Q^T \underline{x} = \underbrace{(\underbrace{Q^T \underline{x}}_{\underline{y}^T})^T}_{\underline{y}^T} \Lambda \underbrace{(Q^T \underline{x})}_{\underline{y}} = \underline{y}^T \Lambda \underline{y} \\
 &= \lambda_1 y_1^2 + \dots + \lambda_n y_n^2. \quad (*)
 \end{aligned}$$

Since Q is orthogonal, there is a one to one correspondence between

all nonzero \pm and nonzero \mp ($y = Q^T \pm$, $\pm = Qy$).

Thus, the values of $q(\pm)$ for $\pm \neq 0$ coincide with the values of (\pm) : the sign of $q(\pm)$ is therefore controlled by the signs of the eigenvalues $\lambda_1, \dots, \lambda_n$ as described in the theorem.

The classification of a quadratic form is used to also classify the matrix k defining it. Thus, a **positive definite matrix** is a symmetric matrix for which the quadratic form $q(\pm) = \pm^T k \pm$ is positive definite, or equivalently, for which all of its eigenvalues are positive (by the theorem above). Equivalent definitions are defined for negative definite, positive/negative semidefinite, and indefinite matrices.

WARNING: The condition that k is positive definite, i.e., that $k > 0$, does NOT mean that all of the entries of k are positive — in fact, many matrices with all positive entries are NOT positive definite!

Example Is $q(x) = 3x_1^2 + 2x_2^2 + x_3^2 + 4x_1x_2 + 4x_2x_3$ a positive definite quadratic form? We construct k as before:

$$q(\pm) = \pm^T k \pm = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \begin{bmatrix} 3 & 2 & 0 \\ 2 & 2 & 2 \\ 0 & 2 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}.$$

$\underbrace{\hspace{10em}}_k$

The eigenvalues of k are 5, 2, and -1, so k is an indefinite matrix, and $q(\pm)$ is an indefinite quadratic form. This is the case even though all entries of k are positive!

Optimization Principles for Eigenvalues of Symmetric Matrices

For symmetric matrices, we've seen that we can interpret eigenvalues as stretching of a vector in the directions specified by the eigenvectors. This is most clearly visualized in terms of a unit ball being mapped to an ellipsoid, as we illustrated earlier.

We can use this observation to answer questions such as what direction is stretched the most by matrix? Or the least? Understanding these questions is essential in areas such as machine learning (which directions are more sensitive to measurement noise or estimation error), control theory (which directions are easiest/hardest to move my system in), and in dimensionality reduction (which directions "explain" most of my data).

These questions all have a flavor of optimization to them: we are looking for directions with the "most" or "least" effect. This motivates a study of eigenvalues of symmetric matrices from an optimization perspective.

We'll start with the simple case of a real diagonal matrix $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n)$. We assume that the diagonal entries, which are the eigenvalues of Λ (why?), appear in decreasing order:

$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n,$$

so that λ_1 is the largest and λ_n is the smallest.

The effect of Λ on a vector y is to multiply its entries by the corresponding diagonal elements: $\Lambda y = (\lambda_1 y_1, \dots, \lambda_n y_n)$. Clearly, the maximal stretch occurs in the e_1 direction, while the minimal (or largest negative) stretch occurs in the e_n direction.

The key idea of the optimization principle for extremal (smallest or biggest) eigenvalues is the following geometric observation. Let's look at the associated quadratic form

$$q(y) = y^T \Lambda y = \lambda_1 y_1^2 + \dots + \lambda_n y_n^2.$$

Suppose that we are asked to pick a vector y on the unit sphere, i.e., a y satisfying $\|y\|^2 = 1$, that makes $q(y)$ as big or small as possible. We can then measure how much/little y has been stretched by looking at the ratio $\frac{q(y)}{\|y\|^2} = q(y) = \|\Lambda^{1/2} y\|^2$.

So let's first look at the maximal direction: this means we are looking for $\|y\|=1$ that maximizes $q(y) = \lambda_1 y_1^2 + \dots + \lambda_n y_n^2$. Since $\lambda_1 \geq \lambda_i$, we have that

$$q(y) = \lambda_1 y_1^2 + \dots + \lambda_n y_n^2 \leq \lambda_1 (y_1^2 + \dots + y_n^2) = \lambda_1$$

and $q(e_1) = \lambda_1$. This means that

$$\lambda_1 = \max \{ q(y) \mid \|y\|=1 \}. \quad (\text{Max})$$

We can use the same reasoning to find that

$$\lambda_n = \min \{ q(y) \mid \|y\|=1 \} \quad (\text{min}).$$

Now, can we make a similar statement for a generic symmetric matrix $K = K^T \in \mathbb{R}^{n \times n}$. Perhaps not surprisingly, using the spectral factorization provides an affirmative answer.

In particular, let $K = Q \Lambda Q^T$ be the spectral factorization of K . Then

$$q(x) = x^T K x = x^T Q \Lambda Q^T x = y^T \Lambda y, \text{ where } y = Q^T x.$$

According to our previous discussion, the maximum of $y^T \Lambda y$ over all unit vectors $\|y\|=1$ is λ_1 , which is the same as the largest eigenvalue of K . Moreover, since Q is an orthogonal matrix, it does not change the length of a vector when it acts on it:

$$1 = \|y\|^2 = y^T y = x^T Q Q^T x = x^T x = \|x\|^2 = 1,$$

so that the maximum of $q(x)$ over all $\|x\|=1$ is again λ_1 . Further, the vector x achieving the maximum is $Q u_1 = u_1$, the corresponding (normalized) eigenvector of K . This is consistent with our prior geometric discussion: the direction with maximal stretch is the vector aligned with the largest semi-axis of the ellipsoid defined by $q(x) = x^T K x = c$, as in Fig. 3(a) above.

We can apply the same reasoning to compute λ_n . We summarize our discussion in the following theorem.

Theorem: Let K be a symmetric matrix with real eigenvalues $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$. Then

$$\lambda_1 = \max \{ x^T K x \mid \|x\|=1 \} \text{ and } \lambda_n = \min \{ x^T K x \mid \|x\|=1 \},$$

are respectively its largest and smallest eigenvalues. The maximal (minimal) value is achieved when $x = \pm u_1$ ($x = \pm u_n$) is one of the unit eigenvectors associated with the largest eigenvalue λ_1 (smallest eigenvalue λ_n).

Example: Maximize the quadratic form $q(x, y) = 3x^2 + 2xy + 3y^2$ over all (x, y) satisfying $x^2 + y^2 = 1$. The quadratic form is defined by the matrix $K = \begin{bmatrix} 3 & 1 \\ 1 & 3 \end{bmatrix}$, which has eigenvalues $\lambda_1 = 4$ and $\lambda_2 = 2$. Therefore

the maximum is $\lambda_1 = 4$, and is achieved at $\begin{bmatrix} x \\ y \end{bmatrix} = \frac{u_1}{\sqrt{2}} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$.

Finally, we note that the above theorem can be generalized to compute general eigenvalues by first eliminating the direction of the larger/smaller eigenvalues. For example, we can compute the second largest eigenvalue of K by solving

$$\lambda_2 = \max \{ x^T K x \mid \|x\|=1, x^T u_1 = 0 \}.$$

The key constraint is $\underline{x}^T \underline{u}_i = 0$, which says we can only look for vectors that are orthogonal to \underline{u}_i , the eigenvector associated with λ_i .

Example: Find the maximum value of $q(x_1, x_2, x_3) = 9x_1^2 + 4x_2^2 + 3x_3^2$ subject to the constraint that $\|\underline{x}\| = 1$ and $\underline{x}^T \underline{u}_1 = 0$, for $\underline{u}_1 = (1, 0, 0)$ the eigenvector corresponding to the greatest eigenvalue $\lambda_1 = 9$ of $K = \text{diag}(9, 4, 3)$. The constraint $\underline{x}^T \underline{u}_1 = 0$ means $x_1 = 0$, and so we need to find (x_2, x_3) satisfying $x_2^2 + x_3^2 = 1$ that maximizes $4x_2^2 + 3x_3^2$. This happens at $(x_2, x_3) = (1, 0)$, leading to a value of 4, which is the second largest eigenvalue λ_2 of K . The corresponding eigenvector is $\underline{u}_2 = (0, 1, 0)$.

ONLINE NOTES: please add a less trivial example and then end with Thm 8.42 from ALA which has the general variational characterization of λ_i .