
Week 13v2

June 5, 2026

Contents

1 Orthogonal Matrices and Symmetric Matrices

Recall that an $n \times n$ matrix A is diagonalizable if and only if it has n linearly independent eigenvectors. Moreover, the matrix P with these eigenvectors as columns is a diagonalizing matrix for A , that is

$$P^{-1}AP = D$$

where D is a diagonal matrix with diagonal entries consisting of the eigenvalues of A .

Orthogonal Matrices

A collection of non-zero, pairwise orthogonal vectors in $\mathbb{R}^n$ is called an *orthogonal* set of vectors. An orthogonal set of vectors is called *orthonormal* if $\|\mathbf{q}\| = 1$ for each vector $\mathbf{q}$ in the set. A set of orthogonal vectors $\{\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k\}$ can be “normalized”, i.e. converted into an orthonormal set $\left\{ \frac{1}{\|\mathbf{v}_1\|} \mathbf{v}_1, \frac{1}{\|\mathbf{v}_2\|} \mathbf{v}_2, \dots, \frac{1}{\|\mathbf{v}_k\|} \mathbf{v}_k \right\}$. In particular, if a matrix A has n orthogonal eigenvectors, they can (by normalizing) be taken to be orthonormal. The corresponding diagonalizing matrix (we will use Q instead of P) has orthonormal columns, and such matrices are very easy to invert.

Theorem 1. The following conditions are equivalent for an $n \times n$ matrix Q .

1. Q is invertible and $Q^{-1} = Q^T$.
2. The rows of Q are orthonormal.
3. The columns of Q are orthonormal.

Proof First note that condition ?? is equivalent to $Q^T Q = I$. Let $\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_n$ denote the columns of Q . Then $\mathbf{q}_i^T$ is the i th row of Q^T , so the (i, j) -entry of $Q^T Q$ is $\mathbf{q}_i \cdot \mathbf{q}_j$. Thus $Q^T Q = I$ means that $\mathbf{q}_i \cdot \mathbf{q}_j = 0$ if $i \neq j$ and $\mathbf{q}_i \cdot \mathbf{q}_i = 1$ if $i = j$. Hence condition ?? is equivalent to ??. The proof of the equivalence of ?? and ?? is similar. ■

Definition 1 (Orthogonal Matrices). An $n \times n$ matrix Q is called an *orthogonal matrix* if its columns are orthonormal vectors. (i.e. The matrix satisfies one (and hence all) of the conditions in Theorem ??.)

Remark 1. The above definition calls a square matrix with orthonormal columns an *orthogonal matrix*. It is true that *orthonormal matrix* might be a better name. But *orthogonal matrix* is standard.

Example 1. The rotation matrix $\begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}$ is orthogonal for any angle θ .

Explanation. See Practice Problem ??.

Exploration 1 Let $A = \begin{bmatrix} 2 & 1 & 1 \\ -1 & 1 & 1 \\ 0 & -1 & 1 \end{bmatrix}$

1. Check that matrix A has rows that are orthogonal.

2. Check that matrix A has columns that are NOT orthogonal.
3. Check that matrix A has rows that are NOT orthonormal.
4. Create a matrix Q by normalizing each of the rows of A .
5. Check that columns and rows of Q are orthonormal.

You should get $Q = \begin{bmatrix} \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ -\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}$.

Definition 2. An $n \times n$ matrix A is said to be *orthogonally diagonalizable* if an orthogonal matrix Q can be found such that $Q^{-1}AQ = Q^T A Q$ is diagonal.

We have learned earlier that when we diagonalize a matrix A , we write $P^{-1}AP = D$ for some matrix P where D is diagonal, and the diagonal entries are the eigenvalues of A . We have also learned that the columns of the matrix P are the corresponding eigenvectors of A . So when a matrix is orthogonally diagonalizable, we are able to accomplish the diagonalization using a matrix Q consisting of n eigenvectors that form an orthonormal basis for $\mathbb{R}^n$. In the following section we will learn that the matrices that have this property are precisely the symmetric matrices.

Symmetric Matrices

A *symmetric matrix* is a matrix which is equal to its transpose.

When we began our study of eigenvalues and eigenvectors, we saw examples of matrices with entries that were real numbers with eigenvalues that were complex numbers. It can be shown that symmetric matrices only have real eigenvalues.

Fact 1. Symmetric matrices only have real eigenvalues.

Lemma 1. If A is an $n \times n$ symmetric matrix, then

$$(Ax) \cdot y = x \cdot (Ay)$$

for all columns x and y in $\mathbb{R}^n$.

Proof Recall that $x \cdot y = x^T y$ for all columns x and y . Because $A^T = A$, we get

$$(Ax) \cdot y = (Ax)^T y = x^T A^T y = x^T A y = x \cdot (Ay)$$

■

Remark 2. The converse of the above lemma also holds (see Practice Problem ??).

Theorem 2. If A is a symmetric matrix, then eigenvectors of A corresponding to distinct eigenvalues are orthogonal.

Proof Let $A\mathbf{x} = \lambda\mathbf{x}$ and $A\mathbf{y} = \mu\mathbf{y}$, where $\lambda \neq \mu$. We compute

$$\lambda(\mathbf{x} \cdot \mathbf{y}) = (\lambda\mathbf{x}) \cdot \mathbf{y} = (A\mathbf{x}) \cdot \mathbf{y} = \mathbf{x} \cdot (A\mathbf{y}) = \mathbf{x} \cdot (\mu\mathbf{y}) = \mu(\mathbf{x} \cdot \mathbf{y})$$

Hence $(\lambda - \mu)(\mathbf{x} \cdot \mathbf{y}) = 0$, and so $\mathbf{x} \cdot \mathbf{y} = 0$ because $\lambda \neq \mu$. ■

Example 2. Find an orthogonal matrix Q such that $Q^{-1}AQ$ is diagonal, where $A = \begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & 2 \\ -1 & 2 & 5 \end{bmatrix}$.

Explanation. The characteristic equation of A is (adding twice row 1 to row 2):

$$\det \begin{bmatrix} 1 - \lambda & 0 & 1 \\ 0 & 1 - \lambda & -2 \\ 1 & -2 & 5 - \lambda \end{bmatrix} = \lambda(\lambda - 1)(\lambda - 6) = 0$$

Thus the eigenvalues are $\lambda = 0, 1$, and 6 , and corresponding eigenvectors are

$$\mathbf{x}_1 = \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix} \quad \mathbf{x}_2 = \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix} \quad \mathbf{x}_3 = \begin{bmatrix} -1 \\ 2 \\ 5 \end{bmatrix}$$

respectively. Moreover, these eigenvectors are *orthogonal*. We have $\|\mathbf{x}_1\|^2 = 6$, $\|\mathbf{x}_2\|^2 = 5$, and $\|\mathbf{x}_3\|^2 = 30$, so

$$P = \begin{bmatrix} \frac{1}{\sqrt{6}}\mathbf{x}_1 & \frac{1}{\sqrt{5}}\mathbf{x}_2 & \frac{1}{\sqrt{30}}\mathbf{x}_3 \end{bmatrix} = \frac{1}{\sqrt{30}} \begin{bmatrix} \sqrt{5} & 2\sqrt{6} & -1 \\ -2\sqrt{5} & \sqrt{6} & 2 \\ \sqrt{5} & 0 & 5 \end{bmatrix}$$

is an orthogonal matrix. Thus $P^{-1} = P^T$ and

$$P^TAP = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 6 \end{bmatrix}.$$

Example 3. Orthogonally diagonalize the symmetric matrix $A = \begin{bmatrix} 8 & -2 & 2 \\ -2 & 5 & 4 \\ 2 & 4 & 5 \end{bmatrix}$.

Explanation. The characteristic equation is

$$\det \begin{bmatrix} 8 - \lambda & 2 & -2 \\ 2 & 5 - \lambda & -4 \\ -2 & -4 & 5 - \lambda \end{bmatrix} = \lambda(\lambda - 9)^2 = 0$$

Hence the distinct eigenvalues are 0 and 9 are of algebraic multiplicity 1 and 2 , respectively. The geometric multiplicities must be the same, for A is diagonalizable, being symmetric. It follows that $\dim(\mathcal{S}_0) = 1$ and $\dim(\mathcal{S}_9) = 2$. Gaussian elimination gives

$$\mathcal{S}_0(A) = \text{span}\{\mathbf{x}_1\}, \quad \mathbf{x}_1 = \begin{bmatrix} 1 \\ 2 \\ -2 \end{bmatrix}, \quad \text{and} \quad \mathcal{S}_9(A) = \text{span} \left\{ \begin{bmatrix} -2 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 2 \\ 0 \\ 1 \end{bmatrix} \right\}$$

The eigenvectors in S_9 are both orthogonal to $\mathbf{x}_1$ as Theorem ?? guarantees, but not to each other. However, an orthogonal basis can be found using projections. (See [Gram-Schmidt Orthogonalization](#))

$$\{\mathbf{f}_2, \mathbf{f}_3\} \text{ of } S_9(A) \quad \text{where} \quad \mathbf{f}_2 = \begin{bmatrix} -2 \\ 1 \\ 0 \end{bmatrix} \quad \text{and} \quad \mathbf{f}_3 = \begin{bmatrix} 2 \\ 4 \\ 5 \end{bmatrix}$$

Normalizing gives orthonormal vectors $\{\frac{1}{3}\mathbf{x}_1, \frac{1}{\sqrt{5}}\mathbf{f}_2, \frac{1}{3\sqrt{5}}\mathbf{f}_3\}$, so

$$Q = \begin{bmatrix} \left| \frac{1}{3}\mathbf{x}_1 \right| & \left| \frac{1}{\sqrt{5}}\mathbf{f}_2 \right| & \left| \frac{1}{3\sqrt{5}}\mathbf{f}_3 \right| \\ \hline \frac{1}{3}\mathbf{x}_1 & \frac{1}{\sqrt{5}}\mathbf{f}_2 & \frac{1}{3\sqrt{5}}\mathbf{f}_3 \\ \hline \end{bmatrix} = \frac{1}{3\sqrt{5}} \begin{bmatrix} \sqrt{5} & -6 & 2 \\ 2\sqrt{5} & 3 & 4 \\ -2\sqrt{5} & 0 & 5 \end{bmatrix}$$

is an orthogonal matrix such that $Q^{-1}AQ$ is diagonal.

It is worth noting that other, more convenient, diagonalizing matrices Q exist. For example, $\mathbf{y}_2 = \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix}$ and $\mathbf{y}_3 = \begin{bmatrix} -2 \\ 2 \\ 1 \end{bmatrix}$

lie in $S_9(A)$ and they are orthogonal. Moreover, they both have norm 3 (as does $\mathbf{x}_1$), so

$$\hat{Q} = \begin{bmatrix} \left| \frac{1}{3}\mathbf{x}_1 \right| & \left| \frac{1}{3}\mathbf{y}_2 \right| & \left| \frac{1}{3}\mathbf{y}_3 \right| \\ \hline \frac{1}{3}\mathbf{x}_1 & \frac{1}{3}\mathbf{y}_2 & \frac{1}{3}\mathbf{y}_3 \\ \hline \end{bmatrix} = \frac{1}{3} \begin{bmatrix} 1 & 2 & -2 \\ 2 & 1 & 2 \\ -2 & 2 & 1 \end{bmatrix}$$

is a nicer orthogonal matrix with the property that $\hat{Q}^{-1}A\hat{Q}$ is diagonal.

Practice Problems

Problem 2 Normalize the columns to make the following matrix orthogonal. $A = \begin{bmatrix} 1 & -4 \\ 2 & 2 \end{bmatrix}$

$$\frac{1}{\sqrt{\dots\dots}} \begin{bmatrix} \dots\dots & \dots\dots \\ \dots\dots & \dots\dots \end{bmatrix}$$

Problem 3 Normalize the columns to make the following matrix orthogonal. $A = \begin{bmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{bmatrix}$

$$\frac{1}{\dots\dots} \begin{bmatrix} \dots\dots & \dots\dots & \dots\dots \\ \dots\dots & \dots\dots & \dots\dots \\ \dots\dots & \dots\dots & \dots\dots \end{bmatrix}$$

Problem 4 For each matrix A , find an orthogonal matrix Q such that $Q^{-1}AQ$ is diagonal.

Question 4.1

$$A = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$Q = \frac{1}{\sqrt{\dots\dots}} \begin{bmatrix} 1 & -1 \\ \dots\dots & \dots\dots \end{bmatrix}$$

Question 4.2

$$A = \begin{bmatrix} 3 & 0 & 7 \\ 0 & 5 & 0 \\ 7 & 0 & 3 \end{bmatrix}$$

List eigenvalues in increasing order.

$$\lambda_1 = \dots\dots, \quad \lambda_2 = \dots\dots, \quad \lambda_3 = \dots\dots$$

$$Q^{-1}AQ = \begin{bmatrix} \dots\dots/\sqrt{\dots\dots} & \dots\dots & \dots\dots/\sqrt{\dots\dots} \\ \dots\dots & \dots\dots & \dots\dots \\ 1/\sqrt{\dots\dots} & \dots\dots & 1/\sqrt{\dots\dots} \end{bmatrix} \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix} \begin{bmatrix} \dots\dots/\sqrt{\dots\dots} & \dots\dots & \dots\dots/\sqrt{\dots\dots} \\ \dots\dots & \dots\dots & \dots\dots \\ 1/\sqrt{\dots\dots} & \dots\dots & 1/\sqrt{\dots\dots} \end{bmatrix}$$

Problem 5 Suppose A is orthogonally diagonalizable. Prove that A is symmetric. (This is the easy direction of the "if and only if" in Theorem ??.)

Problem 6 Prove the converse of Theorem ??:

If $(A\mathbf{x}) \cdot \mathbf{y} = \mathbf{x} \cdot (A\mathbf{y})$ for all n -columns $\mathbf{x}$ and $\mathbf{y}$, then A is symmetric.

Problem 7 Let Q be an orthogonal matrix.

1. Show that $\det Q = 1$ or $\det Q = -1$.
2. Give 2×2 examples of Q such that $\det Q = 1$ and $\det Q = -1$.

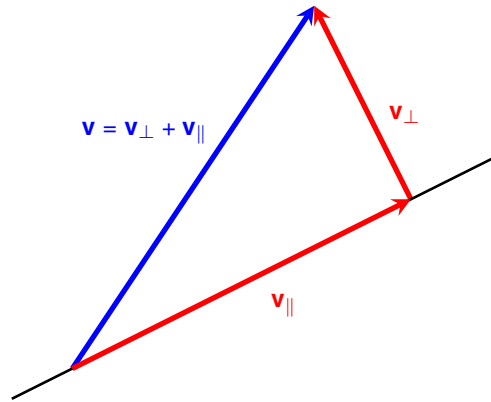
Text Source

This section was adapted from Section 8.2 of Keith Nicholson's *Linear Algebra with Applications*. (CC-BY-NC-SA)

W. Keith Nicholson, *Linear Algebra with Applications*, Lyryx 2018, Open Edition, p. 424

2 Orthogonal Projections

Given a line l and a vector $\mathbf{v}$ emanating from a point on l , it is sometimes convenient to express $\mathbf{v}$ as the sum of a vector $\mathbf{v}_{\parallel}$, parallel to l , and a vector $\mathbf{v}_{\perp}$, perpendicular to l . If you have taken a physics course, you may have seen a force vector decomposed into the sum of two components: one parallel and one perpendicular to the direction of motion.



Suppose $\mathbf{d}$ is a direction vector for l . Then $\mathbf{v}_{\parallel} = k\mathbf{d}$ for some scalar k . Our goal is to find k .

$$\begin{aligned}\mathbf{v} \cdot \mathbf{d} &= (\mathbf{v}_{\parallel} + \mathbf{v}_{\perp}) \cdot \mathbf{d} \\ &= (k\mathbf{d} + \mathbf{v}_{\perp}) \cdot \mathbf{d} \\ &= k\mathbf{d} \cdot \mathbf{d} + \mathbf{v}_{\perp} \cdot \mathbf{d} \\ &= k\|\mathbf{d}\|^2 + 0 \\ &= k\|\mathbf{d}\|^2\end{aligned}$$

We conclude that

$$k = \frac{\mathbf{v} \cdot \mathbf{d}}{\|\mathbf{d}\|^2}$$

and

$$\mathbf{v}_{\parallel} = k\mathbf{d} = \left(\frac{\mathbf{v} \cdot \mathbf{d}}{\|\mathbf{d}\|^2} \right) \mathbf{d}$$

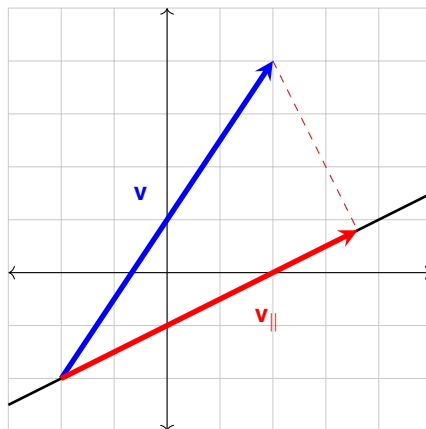
The vector $\mathbf{v}_{\parallel} = \left(\frac{\mathbf{v} \cdot \mathbf{d}}{\|\mathbf{d}\|^2} \right) \mathbf{d}$ is called the *projection of $\mathbf{v}$ onto $\mathbf{d}$* . In our discussion, $\mathbf{d}$ is a direction vector for line l . So, we can also say that $\mathbf{v}_{\parallel}$ is the *projection of $\mathbf{v}$ onto l* .

To find $\mathbf{v}_{\perp}$, observe that $\mathbf{v}_{\perp} = \mathbf{v} - \mathbf{v}_{\parallel}$.

Definition 3. Let $\mathbf{v}$ be a vector, and let $\mathbf{d}$ be a non-zero vector. The *projection of $\mathbf{v}$ onto $\mathbf{d}$* is given by

$$\text{proj}_{\mathbf{d}} \mathbf{v} = \left(\frac{\mathbf{v} \cdot \mathbf{d}}{\|\mathbf{d}\|^2} \right) \mathbf{d}$$

Example 4. Find the projection of $\mathbf{v}$, shown below, onto the line given by $y = \frac{1}{2}x - 1$.



Explanation. We begin by finding vectors $\mathbf{v}$ and $\mathbf{d}$. The tail of $\mathbf{v}$ is located at $(-2, -2)$, and the head of $\mathbf{v}$ is at $(2, 4)$. Using the “head-tail” formula we get

$$\mathbf{v} = \begin{bmatrix} 2 - (-2) \\ 4 - (-2) \end{bmatrix} = \begin{bmatrix} 4 \\ 6 \end{bmatrix}$$

The direction vector for the line $y = \frac{1}{2}x - 1$ is

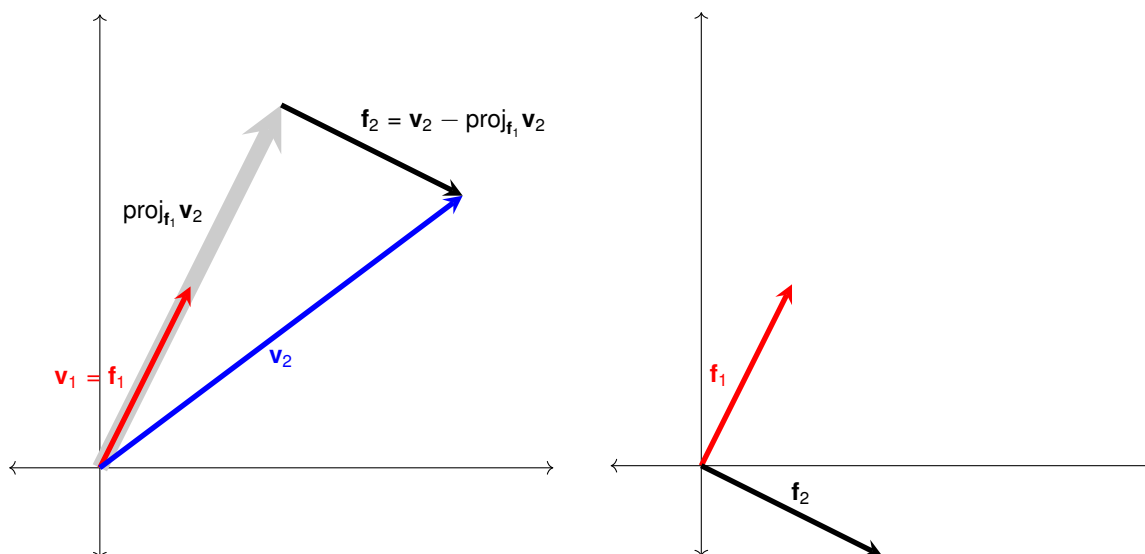
$$\mathbf{d} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$

We find that $\mathbf{v} \cdot \mathbf{d} = 14$ and $\|\mathbf{d}\|^2 = 5$. Thus

$$\text{proj}_{\mathbf{d}} \mathbf{v} = \left(\frac{\mathbf{v} \cdot \mathbf{d}}{\|\mathbf{d}\|^2} \right) \mathbf{d} = \frac{14}{5} \begin{bmatrix} 2 \\ 1 \end{bmatrix} = \begin{bmatrix} 28/5 \\ 14/5 \end{bmatrix}$$

A Visual Guide to Creating an Orthogonal Basis

Given an arbitrary basis $\{\mathbf{v}_1, \mathbf{v}_2\}$ of $\mathbb{R}^2$, let's start building our orthogonal basis, $\{\mathbf{f}_1, \mathbf{f}_2\}$, by setting $\mathbf{f}_1 = \mathbf{v}_1$. To find the next element of our orthogonal basis, consider the orthogonal projection of $\mathbf{v}_2$ onto $\mathbf{f}_1$. (See the figure below.)



Next, let $\mathbf{f}_2 = \mathbf{v}_2 - \text{proj}_{\mathbf{f}_1} \mathbf{v}_2$. Observe that $\mathbf{f}_2$ is orthogonal to $\mathbf{f}_1$ (See Theorem ?? of [Orthogonality and Projections](#)). This gives us an orthogonal collection $\mathcal{B} = \{\mathbf{f}_1, \mathbf{f}_2\}$. It is intuitively clear that $\mathbf{f}_1$ and $\mathbf{f}_2$ are linearly independent. Therefore $\mathcal{B}$ is an orthogonal basis of $\mathbb{R}^2$.

The following exploration illustrates this process dynamically.

Exploration 8 Choose an arbitrary basis $\{\mathbf{v}_1, \mathbf{v}_2\}$ of $\mathbb{R}^2$ by dragging the tips of vectors $\mathbf{v}_1$ and $\mathbf{v}_2$ to desired positions. Use the navigation bar at the bottom of the interactive window to go through the steps of constructing an orthogonal basis of $\mathbb{R}^2$.

Access GeoGebra interactives through the online version of this text at

<https://ximera.osu.edu/linearalgebradv3/LinearAlgebraInteractiveIntro>.

We can apply this process to any two-dimensional subset of $\mathbb{R}^n$. The following exploration will guide you through the process of constructing an orthogonal basis for a plane spanned by two arbitrary vectors in $\mathbb{R}^3$.

Exploration 9 Let $W = \text{span}(\mathbf{v}_1, \mathbf{v}_2)$. W is a plane through the origin in $\mathbb{R}^3$. Use the navigation bar at the bottom of the interactive window to go through the steps of constructing an orthogonal basis for W . RIGHT-CLICK and DRAG to rotate the image for a better view.

Access GeoGebra interactives through the online version of this text at

<https://ximera.osu.edu/linearalgebradv3/LinearAlgebraInteractiveIntro>.

In the next exploration, we take the process of constructing an orthogonal basis to the edge of the visual realm and construct an orthogonal basis for $\mathbb{R}^3$.

Exploration 10 In the GeoGebra interactive below $\{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3\}$ is a basis of $\mathbb{R}^3$. Use check boxes to go through the steps for constructing an orthogonal basis starting with the given basis. RIGHT-CLICK and DRAG to rotate the image for a better view.

Access GeoGebra interactives through the online version of this text at

<https://ximera.osu.edu/linearalgebradv3/LinearAlgebraInteractiveIntro>.

What we saw above are low-dimension examples of what is known as *Gram Schmidt Orthogonalization*.

Practice Problems

Problem 11 Find $\text{proj}_{\mathbf{d}}\mathbf{v}$ if $\mathbf{d} = \begin{bmatrix} -1 \\ 3 \end{bmatrix}$ and $\mathbf{v} = \begin{bmatrix} 1 \\ 4 \end{bmatrix}$.

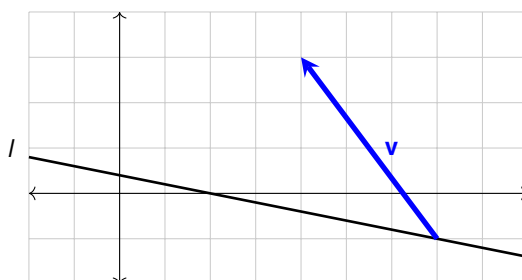
$$\text{proj}_{\mathbf{d}}\mathbf{v} = \begin{bmatrix} \dots \\ \dots \end{bmatrix}$$

Problem 12 Find $\text{proj}_{\mathbf{d}}\mathbf{v}$ if $\mathbf{d} = \begin{bmatrix} 0 \\ 2 \\ 1 \end{bmatrix}$ and $\mathbf{v} = \begin{bmatrix} -1 \\ -4 \\ 2 \end{bmatrix}$.

$$\text{proj}_{\mathbf{d}}\mathbf{v} = \begin{bmatrix} \dots \\ \dots \\ \dots \end{bmatrix}$$

Problem 13 Show that $\text{proj}_{\mathbf{d}}\mathbf{v}$ does not depend on the length of $\mathbf{d}$ by proving that $\text{proj}_{\mathbf{d}}\mathbf{v} = \text{proj}_{k\mathbf{d}}\mathbf{v}$ for $k \neq 0$. What does this result mean geometrically? Illustrate your response with a diagram.

Problem 14 Find the projection of vector $\mathbf{v}$ onto line l . (If entering answers in decimal form, round to the nearest one hundredth.)



Answer:

$$\begin{bmatrix} \dots \\ \dots \end{bmatrix}$$

Problem 15 Convert the given basis $\mathcal{B}$ of $\mathbb{R}^2$ to an orthogonal basis by following the procedure described in this section with $\mathbf{v}_1 = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$.

$$\mathcal{B} = \left\{ \begin{bmatrix} 2 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ -1 \end{bmatrix} \right\}$$

$$\left\{ \begin{bmatrix} 2 \\ 1 \end{bmatrix}, \begin{bmatrix} \dots\dots \\ \dots\dots \end{bmatrix} \right\}$$

3 Least-Squares Approximation

Often an exact solution to a problem in applied mathematics is difficult or impossible to obtain. However, it is usually just as useful to find an approximation to a solution. In particular, finding “linear approximations” is a powerful technique in applied mathematics. One basic case is the situation where a system of linear equations has no solution, and it is desirable to find a “best approximation” to a solution to the system.

We begin by defining the “best approximation” in a natural way, and showing that computing the best approximation reduces to solving a related system of linear equations called the *normal equations*. Next, we demonstrate a common application where a collection of data points is approximated by a line (or a curve). We conclude this section by showing that *QR*-factorization provides us with a more efficient way to solve the normal equations and compute the best approximation.

Best Approximate Solutions

Exploration 16 Let

$$A = \begin{bmatrix} 3 & 1 \\ 1 & 2 \\ 1 & 2 \end{bmatrix} \quad \text{and} \quad \mathbf{b} = \begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix}$$

Consider the matrix equation $A\mathbf{x} = \mathbf{b}$. A quick examination of the last two rows should convince you that this equation has no solutions. In other words, $\mathbf{b}$ is not in the span of the columns of A .

If $\mathbf{z}$ were an exact solution to $A\mathbf{x} = \mathbf{b}$, then $\mathbf{b} - A\mathbf{z}$ would be $\mathbf{0}$. Since the equation does not have a solution, we will attempt to find the next best thing to a solution by finding $\mathbf{z}$ such that $\|\mathbf{b} - A\mathbf{z}\|$ is as small as possible. The quantity $\|\mathbf{b} - A\mathbf{z}\|$ is called the error.

The following GeoGebra interactive will help you understand the geometry behind finding $\mathbf{z}$.

RIGHT-CLICK and DRAG to rotate the image for a better view.

Access GeoGebra interactives through the online version of this text at

<https://ximera.osu.edu/linearalgebradv3/LinearAlgebraInteractiveIntro>.

Record your best guess for $\mathbf{z}$ – you will have a chance to check your answer in Example ??.

What did you discover about the geometry of minimizing $\|\mathbf{b} - A\mathbf{z}\|$? Select all that apply.

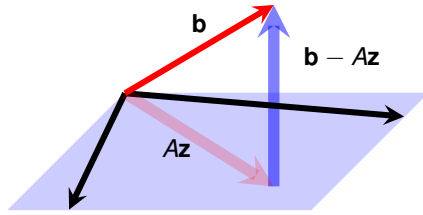
Select All Correct Answers:

1. $\mathbf{z}$ is orthogonal to the plane spanned by the columns of A .
2. $\|\mathbf{b} - A\mathbf{z}\|$ is orthogonal to $\text{col}(A)$.
3. $\mathbf{b} - A\mathbf{z}$ is orthogonal to $\text{col}(A)$.
4. $A\mathbf{z}$ is orthogonal to $\text{col}(A)$.
5. $A\mathbf{z}$ is an orthogonal projection of $\mathbf{b}$ onto $\text{col}(A)$.

Our geometric observations will help us develop a method for finding $\mathbf{z}$.

Suppose A is an $m \times n$ matrix, and $\mathbf{b}$ is a column vector in $\mathbb{R}^m$. Consider the matrix equation $A\mathbf{x} = \mathbf{b}$. If this equation does not have a solution, we can attempt to find a best approximation by finding $\mathbf{z}$ which minimizes the error, $\|\mathbf{b} - A\mathbf{z}\|$. The expression $\|\mathbf{b} - A\mathbf{z}\|$ is also sometimes called the *residual*. The error (or the residual) is given in terms of a vector norm. Recall that our definition of the norm involves the sum of squares of the vector components. When we minimize the norm, we minimize the sum of squares. This is why the method we are describing is often referred to as *least squares*. We will explore this idea further later in this section.

In the case when $\text{col}(A)$ is a subspace of $\mathbb{R}^3$, we can see geometrically that $\mathbf{z}$ is the best approximation if and only if $A\mathbf{z}$ is an orthogonal projection of $\mathbf{b}$ onto $\text{col}(A)$, and the error is the magnitude of $\mathbf{b} - A\mathbf{z}$, as shown below.



What we observed above, holds in general. We will use this fact to find $\mathbf{z}$.

Every vector in $\text{col}(A)$ can be written in the form $A\mathbf{x}$ for some $\mathbf{x}$ in $\mathbb{R}^n$. Our goal is to find $\mathbf{z}$ such that $A\mathbf{z}$ is the orthogonal projection of $\mathbf{b}$ onto $\text{col}(A)$. By Corollary ??, every vector $A\mathbf{x}$ in $\text{col}(A)$ is orthogonal to $\mathbf{b} - A\mathbf{z}$.

Therefore, we have

$$\begin{aligned} A^T(\mathbf{b} - A\mathbf{z}) &= \mathbf{0} \\ A^T\mathbf{b} - A^TA\mathbf{z} &= \mathbf{0} \\ A^TA\mathbf{z} &= A^T\mathbf{b} \end{aligned} \tag{1}$$

Since $\mathbf{b} - A\mathbf{z}$ is normal to the subspace $\text{col}(A)$, we call the system of linear equations in (??) the *normal equations for $\mathbf{z}$* . If A^TA is invertible, then we can write

$$\mathbf{z} = (A^TA)^{-1}A^T\mathbf{b} \tag{2}$$

We will return to the question of invertibility of A^TA in Theorem ??. For now, let's revisit the problem posed in Exploration ??.

Example 5. We now return to the matrix equation $A\mathbf{x} = \mathbf{b}$ of Exploration ?? to find $\mathbf{z}$ that best approximates a solution.

Explanation. Recall that

$$A = \begin{bmatrix} 3 & 1 \\ 1 & 2 \\ 1 & 2 \end{bmatrix} \quad \text{and} \quad \mathbf{b} = \begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix}$$

In this case, $(A^T A)^{-1}$ exists. Applying equation (??), we compute

$$\begin{aligned} \mathbf{z} &= \left(\begin{bmatrix} 3 & 1 & 1 \\ 1 & 2 & 2 \end{bmatrix} \begin{bmatrix} 3 & 1 \\ 1 & 2 \\ 1 & 2 \end{bmatrix} \right)^{-1} \begin{bmatrix} 3 & 1 & 1 \\ 1 & 2 & 2 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix} \\ &= \begin{bmatrix} 11 & 7 \\ 7 & 9 \end{bmatrix}^{-1} \begin{bmatrix} 10 \\ 10 \end{bmatrix} = \begin{bmatrix} 0.18 & -0.14 \\ -0.14 & 0.22 \end{bmatrix} \begin{bmatrix} 10 \\ 10 \end{bmatrix} \\ &= \begin{bmatrix} 0.4 \\ 0.8 \end{bmatrix} \end{aligned}$$

Compare this answer to your guess in Exploration ???. If your guess was correct, nice job! If your guess was different, try setting $\mathbf{z}$ to the correct answer and use the GeoGebra interactive in Exploration ?? to examine the geometry of the problem.

We now come back to the question of when $A^T A$ is invertible.

Theorem 3. If columns of matrix A are linearly independent, then $A^T A$ is invertible.

Proof Let A be a matrix with linearly independent columns. We will show that $(A^T A) \mathbf{x} = \mathbf{0}$ has only the trivial solution. For $\mathbf{x}$, a solution of $A^T A \mathbf{x} = \mathbf{0}$, we have

$$\begin{aligned} \|\mathbf{Ax}\|^2 &= (\mathbf{Ax}) \cdot (\mathbf{Ax}) \\ &= (\mathbf{Ax})^T \mathbf{Ax} \\ &= \mathbf{x}^T A^T \mathbf{Ax} \\ &= \mathbf{x}^T \cdot \mathbf{0} = 0 \end{aligned}$$

Therefore $\mathbf{Ax} = \mathbf{0}$. By linear independence of the columns of A we conclude that $\mathbf{x} = \mathbf{0}$. ■

We summarize our findings in the following theorem.

Theorem 4. Let A be an $m \times n$ matrix, let $\mathbf{b}$ be a column vector in $\mathbb{R}^m$. Consider the matrix equation

$$\mathbf{Ax} = \mathbf{b}$$

1. Any solution $\mathbf{z}$ to the normal equations

$$(A^T A) \mathbf{z} = A^T \mathbf{b}$$

is a best approximation to a solution to $\mathbf{Ax} = \mathbf{b}$ in the sense that $\|\mathbf{b} - \mathbf{Az}\|$ is minimized.

2. If the columns of A are linearly independent, then $A^T A$ is invertible and $\mathbf{z}$ is given uniquely by

$$\mathbf{z} = (A^T A)^{-1} A^T \mathbf{b}$$

Example 6. The system of linear equations

$$\begin{aligned} 3x - y &= 4 \\ x + 2y &= 0 \\ 2x + y &= 1 \end{aligned}$$

has no solution. Find the vector $\mathbf{z}$ that best approximates a solution.

Explanation. We have

$$A = \begin{bmatrix} 3 & -1 \\ 1 & 2 \\ 2 & 1 \end{bmatrix}, \quad \begin{bmatrix} 4 \\ 0 \\ 1 \end{bmatrix}.$$

The normal equations are $(A^T A) \mathbf{z} = A^T \mathbf{b}$. We compute

$$\begin{bmatrix} 3 & 1 & 2 \\ -1 & 2 & 1 \end{bmatrix} \begin{bmatrix} 3 & -1 \\ 1 & 2 \\ 2 & 1 \end{bmatrix} \mathbf{z} = \begin{bmatrix} 3 & 1 & 2 \\ -1 & 2 & 1 \end{bmatrix} \begin{bmatrix} 4 \\ 0 \\ 1 \end{bmatrix}.$$

$$\begin{bmatrix} 14 & 1 \\ 1 & 6 \end{bmatrix} \mathbf{z} = \begin{bmatrix} 14 \\ -3 \end{bmatrix}$$

We observe that $A^T A$ is invertible. Multiplying on the left by $(A^T A)^{-1}$ yields

$$\mathbf{z} = \frac{1}{83} \begin{bmatrix} 87 \\ -56 \end{bmatrix}$$

With this vector $\mathbf{z}$, the left sides of the equations become

$$\begin{aligned} 3(87/83) - (-56/83) &\approx 3.82 \\ (87/83) + 2(-56/83) &\approx -0.30 \\ 2(87/83) + (-56/83) &\approx 1.42 \end{aligned}$$

This is as close as possible to a solution.

Example 7. The average number g of goals per game scored by a hockey player seems to be related linearly to two factors: the number x_1 of years of experience and the number x_2 of goals in the preceding 10 games. The data on the following page were collected on four players. Find the linear function $g = a_0 + a_1 x_1 + a_2 x_2$ that best fits the data.

g	x_1	x_2
0.8	5	3
0.8	3	4
0.6	1	5
0.4	2	1

Explanation. If the relationship is given by $g = a_0 + a_1 x_1 + a_2 x_2$, then the data can be described as follows:

$$\begin{bmatrix} 1 & 5 & 3 \\ 1 & 3 & 4 \\ 1 & 1 & 5 \\ 1 & 2 & 1 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 0.8 \\ 0.8 \\ 0.6 \\ 0.4 \end{bmatrix}$$

Using Theorem ??, we get

$$\mathbf{z} = \frac{1}{42} \underbrace{\begin{bmatrix} 119 & -17 & -19 \\ -17 & 5 & 1 \\ -19 & 1 & 5 \end{bmatrix}}_{(A^T A)^{-1}} \underbrace{\begin{bmatrix} 1 & 1 & 1 & 1 \\ 5 & 3 & 1 & 2 \\ 3 & 4 & 5 & 1 \end{bmatrix}}_{A^T} \begin{bmatrix} 0.8 \\ 0.8 \\ 0.6 \\ 0.4 \end{bmatrix} = \begin{bmatrix} 0.14 \\ 0.09 \\ 0.08 \end{bmatrix}$$

Hence the best-fitting function is $g = 0.14 + 0.09x_1 + 0.08x_2$.

Application of Least Squares to Curve Fitting

In [Curve Fitting](#), we discussed how to fit a function to a set of data points, so that the graph of the function passes through each of the points. We also discussed why doing so is sometimes impossible (two points lie one above the other), and may not even be desirable (overfitting). In this section we will learn how to approximate a collection of data points with a line (or a curve) that fits the “trend” of the points. We will start with data that fit a linear pattern.

Exploration 17 Consider the points $(1, 1)$, $(2, 3)$ and $(4, 4)$. These points do not lie on a straight line, but they have a general upward linear trend. (Typically there would be many more points to consider, but we will limit our exploration to what we can do by hand.) Our goal is to find a line that fits these points as closely as possible.

We are looking for a function f of the form $f(x) = ax + b$ such that the following infeasible system is satisfied as closely as possible

$$\begin{aligned} a(1) + b &= 1 \\ a(2) + b &= 3 \\ a(4) + b &= 4 \end{aligned}$$

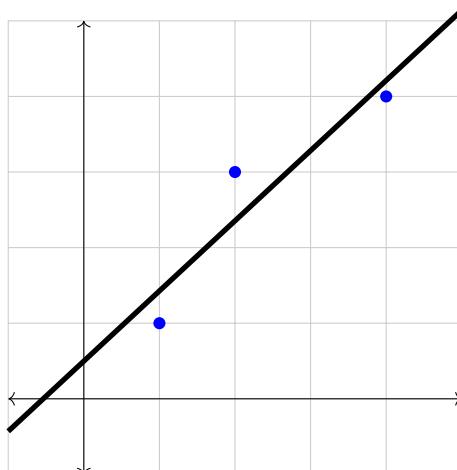
From the first part of this section we know how to find a best approximation. By Theorem ??, we have

$$\begin{aligned} \mathbf{z} = \begin{bmatrix} a \\ b \end{bmatrix} &= (A^T A)^{-1} A^T \mathbf{b} \\ &= \left(\begin{bmatrix} 1 & 2 & 4 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 2 & 1 \\ 4 & 1 \end{bmatrix} \right)^{-1} \begin{bmatrix} 1 & 2 & 4 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 3 \\ 4 \end{bmatrix} \\ &= \begin{bmatrix} 13/14 \\ 1/2 \end{bmatrix} \end{aligned}$$

According to our computations, the line that best fits the data is given by

$$f(x) = \frac{13}{14}x + \frac{1}{2}$$

Let's take a look.



We found this fit by minimizing $\|\mathbf{b} - \mathbf{Az}\|$. We will now investigate the meaning of this expression in relation to the line and the data points.

$$\mathbf{b} - \mathbf{Az} = \begin{bmatrix} 1 \\ 3 \\ 4 \end{bmatrix} - \begin{bmatrix} (13/14)(1) + 1/2 \\ (13/14)(2) + 1/2 \\ (13/14)(4) + 1/2 \end{bmatrix} \approx \begin{bmatrix} -0.43 \\ 0.64 \\ -0.21 \end{bmatrix} \quad (3)$$

Observe that each entry of $\mathbf{b} - \mathbf{Az}$ is the signed vertical distance between a particular point and the line.

Instead of computing the error, $\|\mathbf{b} - \mathbf{Az}\|$, we will compute $\|\mathbf{b} - \mathbf{Az}\|^2$ to avoid the square root.

$$\|\mathbf{b} - \mathbf{Az}\|^2 = (-0.43)^2 + 0.64^2 + (-0.21)^2 \approx 0.64 \quad (4)$$

Minimizing $\|\mathbf{b} - \mathbf{Az}\|$ also minimizes $\|\mathbf{b} - \mathbf{Az}\|^2$. Therefore, what we have minimized is the sum of squares of the vertical distances between the data points and the line. The following GeoGebra interactive will help you explore this idea.

Access GeoGebra interactives through the online version of this text at

<https://ximera.osu.edu/linearalgebradv3/LinearAlgebraInteractiveIntro>.

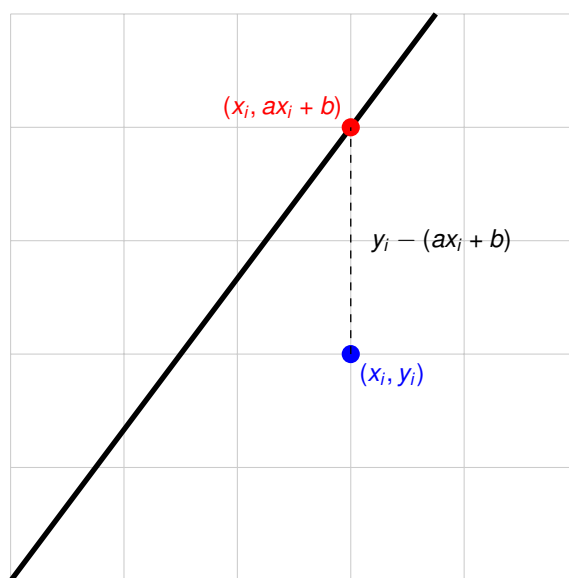
In Exploration ?? we discovered that $\|\mathbf{b} - \mathbf{Az}\|^2$ is the sum of squares of vertical distances between the given data points and the proposed line. By minimizing $\|\mathbf{b} - \mathbf{Az}\|$, we minimize the sum of squares of vertical distances. This observation holds in general. Given a collection of points $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$, finding a linear function of the form $f(x) = ax + b$ that best fits the points we would find a best solution to the system

$$\begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

by minimizing

$$\left\| \begin{bmatrix} y_1 - (ax_1 + b) \\ y_2 - (ax_2 + b) \\ \vdots \\ y_n - (ax_n + b) \end{bmatrix} \right\|^2 = (y_1 - (ax_1 + b))^2 + (y_2 - (ax_2 + b))^2 + \cdots + (y_n - (ax_n + b))^2$$

A geometric interpretation of $y_i - (ax_i + b)$ is shown below.



The line we obtain in this fashion is called a *line of best fit* or a *trendline*, and the method we used is referred to as the *method of least squares*.

We can apply the method of least squares to find best fitting non-linear functions.

Example 8. Find the least squares approximating quadratic polynomial of the form $f(x) = ax^2 + bx + c$ for the following points.

$$(-3, 3), (-1, 1), (0, 1), (1, 2), (3, 4)$$

Explanation. We are looking for an approximate solution to the system of equations

$$\begin{aligned} a(-3)^2 + b(-3) + c &= 3 \\ a(-1)^2 + b(-1) + c &= 1 \\ a(0)^2 + b(0) + c &= 1 \\ a(1)^2 + b(1) + c &= 2 \\ a(3)^2 + b(3) + c &= 4 \end{aligned}$$

This corresponds to the matrix equation

$$\begin{bmatrix} 9 & -3 & 1 \\ 1 & -1 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 1 \\ 9 & 3 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 3 \\ 1 \\ 1 \\ 2 \\ 4 \end{bmatrix}$$

Multiplying on the left by A^T gives us the normal equations.

$$A^T A \mathbf{z} = A^T \mathbf{b}$$

$$\begin{bmatrix} 164 & 0 & 20 \\ 0 & 20 & 0 \\ 20 & 0 & 5 \end{bmatrix} \mathbf{z} = \begin{bmatrix} 66 \\ 11 \\ 4 \end{bmatrix}$$

It turns out that $A^T A$ is invertible, so it is easy to solve for $\mathbf{z}$. You can use technology to accomplish this.

We arrive at the solution

$$\mathbf{z} = \begin{bmatrix} 0.26 \\ 0.20 \\ 1.15 \end{bmatrix}$$

Therefore, the quadratic function of best fit is given by $f(x) = 0.26x^2 + 0.2x + 1.15$. You can see the graph and the points shown below.

For more information about doing least squares with Octave, please see [Octave for Chapter 9](#).

Example 9. Given the data points $(-1, 0)$, $(0, 1)$, and $(1, 4)$, find the least squares approximating function of the form $f(x) = ax + b2^x$.

Explanation. We are looking for an approximate solution to the system of equations

$$\begin{aligned} a(-1) + b(2^{-1}) &= 0 \\ a(0) + b(2^0) &= 1 \\ a(1) + b(2^1) &= 4 \end{aligned}$$

This corresponds to the matrix equation

$$\begin{bmatrix} -1 & 1/2 \\ 0 & 1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 4 \end{bmatrix}$$

Using the normal equations, we obtain

$$A^T A \mathbf{z} = A^T \mathbf{b}$$

$$\frac{1}{4} \begin{bmatrix} 8 & 6 \\ 6 & 21 \end{bmatrix} \mathbf{z} = \begin{bmatrix} 4 \\ 9 \end{bmatrix}$$

Solving for $\mathbf{z}$ yields

$$\mathbf{z} = \begin{bmatrix} 10/11 \\ 16/11 \end{bmatrix}$$

Therefore, the function of best fit (of the given form) is given by

$$f(x) = \frac{10}{11}x + \frac{16}{11}(2^x)$$

Practice Problems

Problem 18 Find the best approximation to a solution to the system of equations.

$$\begin{array}{rrcr} 3x & + & y & + & z & = & 6 \\ 2x & + & 3y & - & z & = & 1 \\ 2x & - & y & + & z & = & 0 \\ 3x & - & 3y & + & 3z & = & 8 \end{array}$$

Enter answers in fraction form below.

$$x = \dots\dots, \quad y = \dots\dots, \quad z = \dots\dots$$

Problem 19 Find a linear function of best fit for the given set of data points. Examine how well your line fits the points by typing the equation of the line into the Desmos window.

$$(2, 4), (4, 3), (7, 2), (8, 1)$$

Enter your answers in fraction form.

$$f(x) = \dots\dots x + \dots\dots$$

Problem 20 Find a linear function of best fit for the given set of data points. Examine how well your line fits the points by typing the equation of the line into the Desmos window.

$$(-2, 3), (-1, 1), (0, 0), (1, -2), (2, -4)$$

$$f(x) = \dots\dots x + \dots\dots$$

Problem 21 Use Octave to find the least squares approximating quadratic function for the following data points.

$$(-2, 1), (0, 0), (3, 2), (4, 3)$$

Round your answers to three decimal places.

$$f(x) = \dots\dots x^2 + \dots\dots x + \dots\dots$$

For more information about doing least squares with Octave, please see [Octave for Chapter 9](#).

Text Source

A portion of this section has been adapted from W. Keith Nicholson, *Linear Algebra with Applications*, Lyryx 2021-A, Open Edition, pp. 308-319.