Chapter 4

Orthogonality

4.1 Orthogonality of the Four Subspaces

1 Orthogonal vectors have $\boldsymbol{v}^{\mathrm{T}}\boldsymbol{w} = 0$. Then $||\boldsymbol{v}||^2 + ||\boldsymbol{w}||^2 = ||\boldsymbol{v}+\boldsymbol{w}||^2 = ||\boldsymbol{v}-\boldsymbol{w}||^2$.

2 Subspaces $\boldsymbol{V}$ and $\boldsymbol{W}$ are orthogonal when $\boldsymbol{v}^{\mathrm{T}}\boldsymbol{w} = 0$ for every $\boldsymbol{v}$ in $\boldsymbol{V}$ and every $\boldsymbol{w}$ in $\boldsymbol{W}$.

3 The row space of A is orthogonal to the nullspace. The column space is orthogonal to $\boldsymbol{N}(A^{\mathrm{T}})$.

4 One pair of dimensions adds to $r + (n - r) = n$. The other pair has $r + (m - r) = m$.

5 Row space and nullspace are orthogonal *complements*: Every $\boldsymbol{x}$ in $\mathbf{R}^n$ splits into $\boldsymbol{x}_{\mathbf{row}} + \boldsymbol{x}_{\mathbf{null}}$.

6 Suppose a space $\boldsymbol{S}$ has dimension d. Then every basis for $\boldsymbol{S}$ consists of d vectors.

7 If d vectors in $\boldsymbol{S}$ are independent, they span $\boldsymbol{S}$. If d vectors span $\boldsymbol{S}$, they are independent.

Two vectors are orthogonal when their dot product is zero: $\boldsymbol{v} \cdot \boldsymbol{w} = \boldsymbol{v}^{\mathrm{T}}\boldsymbol{w} = 0$. This chapter moves to **orthogonal subspaces** and **orthogonal bases** and **orthogonal matrices**. The vectors in two subspaces, and the vectors in a basis, and the column vectors in Q, all pairs will be orthogonal. Think of $a^2 + b^2 = c^2$ for a *right triangle* with sides $\boldsymbol{v}$ and $\boldsymbol{w}$.

Orthogonal vectors $\quad \boldsymbol{v}^{\mathrm{T}}\boldsymbol{w} = 0 \quad$ and $\quad ||\boldsymbol{v}||^2 + ||\boldsymbol{w}||^2 = ||\boldsymbol{v}+\boldsymbol{w}||^2$.

The right side is $(\boldsymbol{v}+\boldsymbol{w})^{\mathrm{T}}(\boldsymbol{v}+\boldsymbol{w})$. This equals $\boldsymbol{v}^{\mathrm{T}}\boldsymbol{v} + \boldsymbol{w}^{\mathrm{T}}\boldsymbol{w}$ when $\boldsymbol{v}^{\mathrm{T}}\boldsymbol{w} = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{v} = 0$.

Subspaces entered Chapter 3 to throw light on $A\boldsymbol{x} = \boldsymbol{b}$. Right away we needed the column space and the nullspace. Then the light turned onto A^{T}, uncovering two more subspaces. Those four fundamental subspaces reveal what a matrix really does.

A matrix multiplies a vector: A *times* $\boldsymbol{x}$. At the first level this is only numbers. At the second level $A\boldsymbol{x}$ is a combination of column vectors. The third level shows subspaces. But I don't think you have seen the whole picture until you study Figure 4.2.

The subspaces fit together to show the hidden reality of A times x. The $90°$ angles between subspaces are new—and we can say now what those right angles mean.

The row space is perpendicular to the nullspace. Every row of A is perpendicular to every solution of $A\boldsymbol{x} = \mathbf{0}$. That gives the $90°$ angle on the left side of the figure. This perpendicularity of subspaces is Part 2 of the Fundamental Theorem of Linear Algebra.

The column space is perpendicular to the nullspace of A^{T}. When $\boldsymbol{b}$ is outside the column space—when we want to solve $A\boldsymbol{x} = \boldsymbol{b}$ and can't do it—then this nullspace of A^{T} comes into its own. It contains the error $\boldsymbol{e} = \boldsymbol{b} - A\boldsymbol{x}$ in the "least-squares" solution. Least squares is the key application of linear algebra in this chapter.

Part 1 of the Fundamental Theorem gave the dimensions of the subspaces. The row and column spaces have the same dimension r (they are drawn the same size). The two nullspaces have the remaining dimensions $n - r$ and $m - r$. Now we will show that ***the row space and nullspace are orthogonal subspaces inside*** $\mathbf{R}^n$.

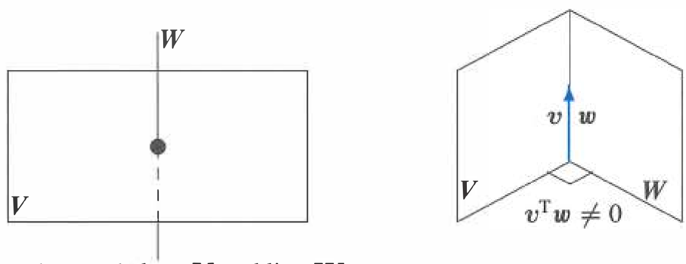
DEFINITION Two subspaces $\boldsymbol{V}$ and $\boldsymbol{W}$ of a vector space are ***orthogonal*** if every vector $\boldsymbol{v}$ in $\boldsymbol{V}$ is perpendicular to every vector $\boldsymbol{w}$ in $\boldsymbol{W}$:

Orthogonal subspaces $\quad v^{\mathrm{T}}w = 0$ ***for all v in V and all w in W.***

Example 1 The floor of your room (extended to infinity) is a subspace $\boldsymbol{V}$. The line where two walls meet is a subspace $\boldsymbol{W}$ (one-dimensional). Those subspaces are orthogonal. Every vector up the meeting line of the walls is perpendicular to every vector in the floor.

Example 2 Two walls look perpendicular but those two subspaces are not orthogonal! The meeting line is in both $\boldsymbol{V}$ and $\boldsymbol{W}$—and this line is not perpendicular to itself. Two planes (dimensions 2 and 2 in $\mathbf{R}^3$) cannot be orthogonal subspaces.

When a vector is in two orthogonal subspaces, it *must* be zero. It is perpendicular to itself. It is $\boldsymbol{v}$ and it is $\boldsymbol{w}$, so $\boldsymbol{v}^{\mathrm{T}}\boldsymbol{v} = 0$. This has to be the zero vector.



orthogonal plane $\boldsymbol{V}$ and line $\boldsymbol{W}$ non-orthogonal planes

Figure 4.1: Orthogonality is impossible when $\dim \boldsymbol{V} + \dim \boldsymbol{W} > \dim$ (whole space).

The crucial examples for linear algebra come from the four fundamental subspaces. Zero is the only point where the nullspace meets the row space. More than that, the **nullspace and row space of A meet at $90°$**. This key fact comes directly from $A\boldsymbol{x} = \mathbf{0}$:

Every vector $\boldsymbol{x}$ in the nullspace is perpendicular to every row of A, because $A\boldsymbol{x} = \mathbf{0}$. ***The nullspace*** $\boldsymbol{N}(A)$ ***and the row space*** $\boldsymbol{C}(A^{\mathrm{T}})$ ***are orthogonal subspaces of*** $\mathbf{R}^n$.

To see why $\boldsymbol{x}$ is perpendicular to the rows, look at $A\boldsymbol{x} = \mathbf{0}$. Each row multiplies $\boldsymbol{x}$:

$$A\boldsymbol{x} = \begin{bmatrix} \textbf{row 1} \\ \vdots \\ \textbf{row } m \end{bmatrix} \begin{bmatrix} \\ \boldsymbol{x} \\ \\ \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix} \quad \begin{matrix} \longleftarrow & (\textbf{row 1}) \cdot \boldsymbol{x} \text{ is zero} \\ \\ \longleftarrow & (\textbf{row } m) \cdot \boldsymbol{x} \text{ is zero} \end{matrix} \tag{1}$$

The first equation says that row 1 is perpendicular to $\boldsymbol{x}$. The last equation says that row m is perpendicular to $\boldsymbol{x}$. *Every row has a zero dot product with* $\boldsymbol{x}$. Then $\boldsymbol{x}$ is also perpendicular to every *combination* of the rows. The whole row space $\boldsymbol{C}(A^{\mathrm{T}})$ is orthogonal to $\boldsymbol{N}(A)$.

Here is a second proof of that orthogonality for readers who like matrix shorthand. The vectors in the row space are combinations $A^{\mathrm{T}}\boldsymbol{y}$ of the rows. Take the dot product of $A^{\mathrm{T}}\boldsymbol{y}$ with any $\boldsymbol{x}$ in the nullspace. *These vectors are perpendicular*:

Nullspace orthogonal to row space $\qquad \boldsymbol{x}^{\mathrm{T}}(A^{\mathrm{T}}\boldsymbol{y}) = (A\boldsymbol{x})^{\mathrm{T}}\boldsymbol{y} = \mathbf{0}^{\mathrm{T}}\boldsymbol{y} = 0. \qquad (2)$

We like the first proof. You can see those rows of A multiplying $\boldsymbol{x}$ to produce zeros in equation (1). The second proof shows why A and A^{T} are both in the Fundamental Theorem.

Example 3 The rows of A are perpendicular to $\boldsymbol{x} = (1, 1, -1)$ in the nullspace:

$$A\boldsymbol{x} = \begin{bmatrix} 1 & 3 & 4 \\ 5 & 2 & 7 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \text{gives the dot products} \quad \begin{matrix} 1 + 3 - 4 = 0 \\ 5 + 2 - 7 = 0 \end{matrix}$$

Now we turn to the other two subspaces. In this example, the column space is all of $\mathbf{R}^2$. The nullspace of A^{T} is only the zero vector (orthogonal to every vector). The column space of A and the nullspace of A^{T} are always orthogonal subspaces.

Every vector $\boldsymbol{y}$ in the nullspace of A^{T} is perpendicular to every column of A. ***The left nullspace*** $\boldsymbol{N}(A^{\mathrm{T}})$ ***and the column space*** $\boldsymbol{C}(A)$ ***are orthogonal in*** $\mathbf{R}^m$.

Apply the original proof to A^{T}. The nullspace of A^{T} is orthogonal to the row space of A^{T}—and the row space of A^{T} is the column space of A. Q.E.D.

For a visual proof, look at $A^{\mathrm{T}}\boldsymbol{y} = \mathbf{0}$. Each column of A multiplies $\boldsymbol{y}$ to give 0:

$$\boldsymbol{C}(\boldsymbol{A}) \perp \boldsymbol{N}(\boldsymbol{A}^{\mathrm{T}}) \qquad A^{\mathrm{T}}\boldsymbol{y} = \begin{bmatrix} (\textbf{column 1})^{\mathrm{T}} \\ \cdots \\ (\textbf{column } n)^{\mathrm{T}} \end{bmatrix} \begin{bmatrix} \\ \boldsymbol{y} \\ \\ \end{bmatrix} = \begin{bmatrix} 0 \\ \cdot \\ 0 \end{bmatrix}. \tag{3}$$

The dot product of $\boldsymbol{y}$ with every column of A is zero. Then $\boldsymbol{y}$ in the left nullspace is perpendicular to each column of A—and to the whole column space.

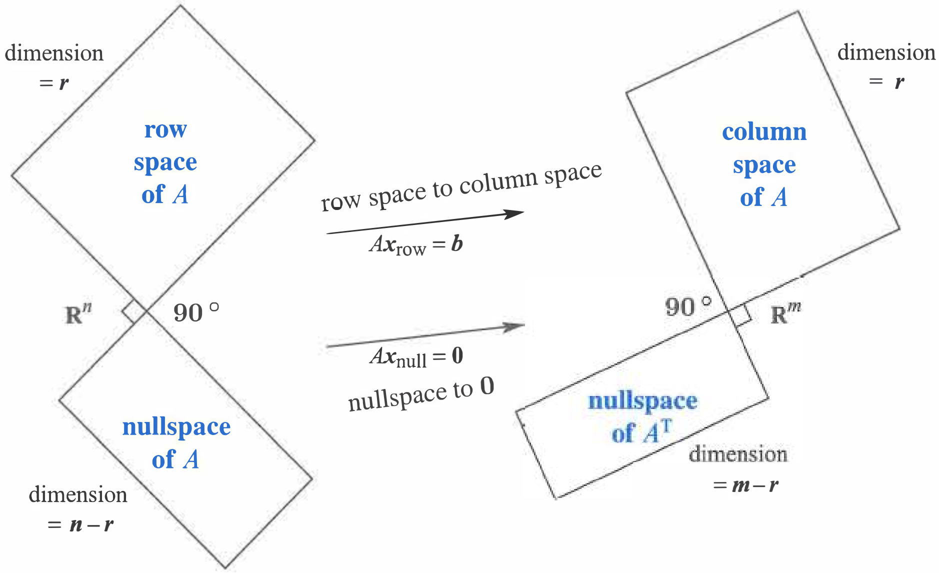


Figure 4.2: Two pairs of orthogonal subspaces. The dimensions add to n and add to m. **This is the Big Picture**—two subspaces in $\mathbf{R}^n$ and two subspaces in $\mathbf{R}^m$.

Orthogonal Complements

Important The fundamental subspaces are more than just orthogonal (in pairs). Their dimensions are also right. Two lines could be perpendicular in $\mathbf{R}^3$, **but those lines *could not be* the row space and nullspace of a 3 by 3 matrix**. The lines have dimensions 1 and 1, adding to 2. But the correct dimensions r and $n - r$ must add to $n = 3$.

The fundamental subspaces of a 3 by 3 matrix have dimensions 2 and 1, or 3 and 0. Those pairs of subspaces are not only orthogonal, they are *orthogonal complements*.

DEFINITION The ***orthogonal complement*** of a subspace $\boldsymbol{V}$ contains ***every*** vector that is perpendicular to $\boldsymbol{V}$. This orthogonal subspace is denoted by $\boldsymbol{V}^{\perp}$ (pronounced "$\boldsymbol{V}$ perp").

By this definition, the nullspace is the orthogonal complement of the row space. ***Every*** $\boldsymbol{x}$ that is perpendicular to the rows satisfies $A\boldsymbol{x} = \mathbf{0}$, and lies in the nullspace.

The reverse is also true. ***If $\boldsymbol{v}$ is orthogonal to the nullspace, it must be in the row space***. Otherwise we could add this $\boldsymbol{v}$ as an extra row of the matrix, without changing its nullspace. The row space would grow, which breaks the law $r + (n - r) = n$. We conclude that the nullspace complement $\boldsymbol{N}(A)^{\perp}$ is exactly the row space $\boldsymbol{C}(A^{\mathrm{T}})$.

In the same way, the left nullspace and column space are orthogonal in $\mathbf{R}^m$, and they are orthogonal complements. Their dimensions r and $m - r$ add to the full dimension m.

Fundamental Theorem of Linear Algebra, Part 2

$N(A)$ is the orthogonal complement of the row space $C(A^{\mathrm{T}})$ (in $\mathbf{R}^n$).

$N(A^{\mathrm{T}})$ is the orthogonal complement of the column space $C(A)$ (in $\mathbf{R}^m$).

Part 1 gave the dimensions of the subspaces. Part 2 gives the 90° angles between them. The point of "complements" is that every $\boldsymbol{x}$ can be split into a *row space component* $\boldsymbol{x}_r$ and a *nullspace component* $\boldsymbol{x}_n$. When A multiplies $\boldsymbol{x} = \boldsymbol{x}_r + \boldsymbol{x}_n$, Figure 4.3 shows what happens to $A\boldsymbol{x} = A\boldsymbol{x}_r + A\boldsymbol{x}_n$:

The nullspace component goes to zero: $A\boldsymbol{x}_n = \mathbf{0}$.

The row space component goes to the column space: $A\boldsymbol{x}_r = A\boldsymbol{x}$.

Every vector goes to the column space! Multiplying by A cannot do anything else. More than that: *Every vector $\boldsymbol{b}$ in the column space comes from one and only one vector $\boldsymbol{x}_r$ in the row space.* Proof: If $A\boldsymbol{x}_r = A\boldsymbol{x}'_r$, the difference $\boldsymbol{x}_r - \boldsymbol{x}'_r$ is in the nullspace. It is also in the row space, where $\boldsymbol{x}_r$ and $\boldsymbol{x}'_r$ came from. This difference must be the zero vector, because the nullspace and row space are perpendicular. Therefore $\boldsymbol{x}_r = \boldsymbol{x}'_r$.

There is an r by r invertible matrix hiding inside A, if we throw away the two nullspaces. ***From the row space to the column space, A is invertible***. The "pseudoinverse" will invert that part of A in Section 7.4.

Example 4 Every matrix of rank r has an r by r invertible submatrix:

$$A = \begin{bmatrix} 3 & 0 & 0 & 0 & 0 \\ 0 & 5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad \text{contains the submatrix} \quad \begin{bmatrix} 3 & 0 \\ 0 & 5 \end{bmatrix}.$$

The other eleven zeros are responsible for the nullspaces. The rank of B is also $r = 2$:

$$B = \begin{bmatrix} 1 & 2 & 3 & 4 & 5 \\ 1 & 2 & 4 & 5 & 6 \\ 1 & 2 & 4 & 5 & 6 \end{bmatrix} \quad \text{contains} \quad \begin{bmatrix} 1 & 3 \\ 1 & 4 \end{bmatrix} \quad \text{in the pivot rows and columns.}$$

Every matrix can be diagonalized, when we choose the right bases for $\mathbf{R}^n$ and $\mathbf{R}^m$. This ***Singular Value Decomposition*** has become extremely important in applications.

Let me repeat one clear fact. A row of A can't be in the nullspace of A (except for a zero row). The only vector in two orthogonal subspaces is the zero vector.

If a vector v is orthogonal to itself then v is the zero vector.

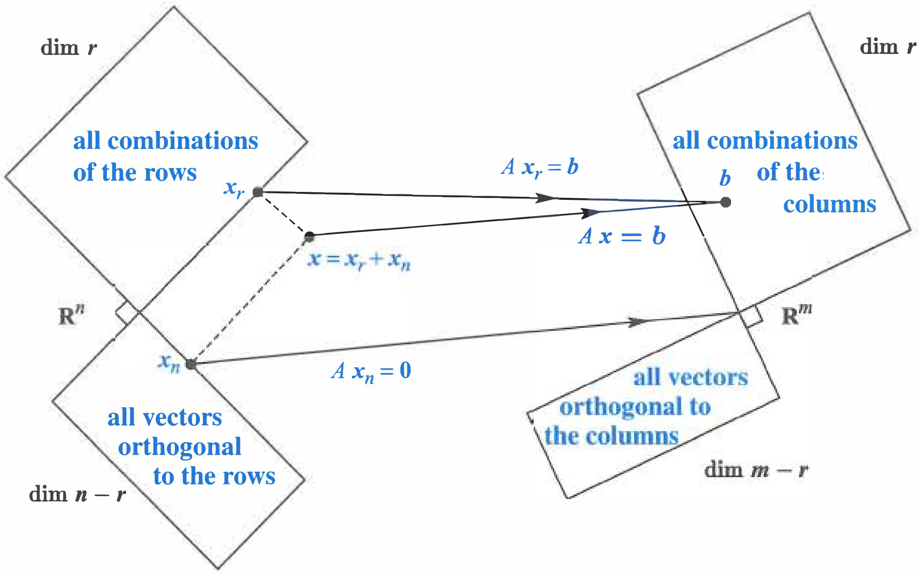


Figure 4.3: This update of Figure 4.2 shows the true action of A on $\boldsymbol{x} = \boldsymbol{x}_r + \boldsymbol{x}_n$. Row space vector $\boldsymbol{x}_r$ to column space, nullspace vector $\boldsymbol{x}_n$ to zero.

Drawing the Big Picture

I don't know the best way to draw the four subspaces in Figures 4.2 and 4.3. This big picture has to show the orthogonality of those subspaces. I can see a possible way to do it when a line meets a plane—maybe Figure 4.4 also shows that those spaces are infinite, more clearly than the rectangles in Figure 4.3. But how do I draw a pair of two-dimensional subspaces in $\mathbf{R}^4$, to show they are orthogonal to each other? Good ideas are welcome.

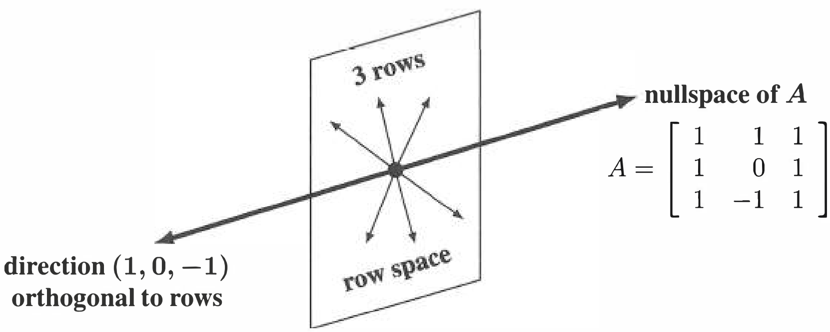


Figure 4.4: Row space of A = plane. Nullspace = orthogonal line. Dimensions $2 + 1 = 3$.

Combining Bases from Subspaces

What follows are some valuable facts about bases. They were saved until now—when we are ready to use them. After a week you have a clearer sense of what a basis is (*linearly independent* vectors that *span the space*). Normally we have to check both properties. When the count is right, one property implies the other:

> Any n independent vectors in $\mathbf{R}^n$ must span $\mathbf{R}^n$. So they are a basis.
> Any n vectors that span $\mathbf{R}^n$ must be independent. So they are a basis.

Starting with the correct number of vectors, one property of a basis produces the other. This is true in any vector space, but we care most about $\mathbf{R}^n$. When the vectors go into the columns of an n by n *square* matrix A, here are the same two facts:

> If the n columns of A are independent, they span $\mathbf{R}^n$. So $A\boldsymbol{x} = \boldsymbol{b}$ is solvable.
> If the n columns span $\mathbf{R}^n$, they are independent. So $A\boldsymbol{x} = \boldsymbol{b}$ has only one solution.

Uniqueness implies existence and existence implies uniqueness. ***Then A is invertible***. If there are no free variables, the solution $\boldsymbol{x}$ is unique. There must be n pivot columns. Then back substitution solves $A\boldsymbol{x} = \boldsymbol{b}$ (the solution exists).

Starting in the opposite direction, suppose that $A\boldsymbol{x} = \boldsymbol{b}$ can be solved for every $\boldsymbol{b}$ (*existence of solutions*). Then elimination produced no zero rows. There are n pivots and no free variables. The nullspace contains only $\boldsymbol{x} = \mathbf{0}$ (*uniqueness* of solutions).

With bases for the row space and the nullspace, we have $r + (n - r) = n$ vectors. This is the right number. Those n vectors are independent.[2] *Therefore they span* $\mathbf{R}^n$.

Each $\boldsymbol{x}$ is the sum $\boldsymbol{x}_r + \boldsymbol{x}_n$ of a row space vector $\boldsymbol{x}_r$ and a nullspace vector $\boldsymbol{x}_n$.

The splitting in Figure 4.3 shows the key point of orthogonal complements—the dimensions add to n and all vectors are fully accounted for.

Example 5 For $A = \begin{bmatrix} 1 & 2 \\ 3 & 6 \end{bmatrix}$ split $\boldsymbol{x} = \begin{bmatrix} 4 \\ 3 \end{bmatrix}$ into $\boldsymbol{x}_r + \boldsymbol{x}_n = \begin{bmatrix} 2 \\ 4 \end{bmatrix} + \begin{bmatrix} 2 \\ -1 \end{bmatrix}$.

The vector $(2, 4)$ is in the row space. The orthogonal vector $(2, -1)$ is in the nullspace. The next section will compute this splitting for any A and $\boldsymbol{x}$, by a projection.

[2] If a combination of all n vectors gives $\boldsymbol{x}_r + \boldsymbol{x}_n = \mathbf{0}$, then $\boldsymbol{x}_r = -\boldsymbol{x}_n$ is in both subspaces. So $\boldsymbol{x}_r = \boldsymbol{x}_n = \mathbf{0}$. All coefficients of the row space basis and of the nullspace basis must be zero. This proves independence of the n vectors together.

■ REVIEW OF THE KEY IDEAS ■

1. Subspaces $\boldsymbol{V}$ and $\boldsymbol{W}$ are orthogonal if every $\boldsymbol{v}$ in $\boldsymbol{V}$ is orthogonal to every $\boldsymbol{w}$ in $\boldsymbol{W}$.

2. $\boldsymbol{V}$ and $\boldsymbol{W}$ are "orthogonal complements" if $\boldsymbol{W}$ contains **all** vectors perpendicular to $\boldsymbol{V}$ (and vice versa). Inside $\mathbf{R}^n$, the dimensions of complements $\boldsymbol{V}$ and $\boldsymbol{W}$ add to n.

3. The nullspace $\boldsymbol{N}(A)$ and the row space $\boldsymbol{C}(A^{\mathrm{T}})$ are orthogonal complements, with dimensions $(n-r)+r=n$. Similarly $\boldsymbol{N}(A^{\mathrm{T}})$ and $\boldsymbol{C}(A)$ are orthogonal complements with $(m-r)+r=m$.

4. Any n independent vectors in $\mathbf{R}^n$ span $\mathbf{R}^n$. Any n spanning vectors are independent.

■ WORKED EXAMPLES ■

4.1 A Suppose $\boldsymbol{S}$ is a six-dimensional subspace of nine-dimensional space $\mathbf{R}^9$.

(a) What are the possible dimensions of subspaces orthogonal to $\boldsymbol{S}$?

(b) What are the possible dimensions of the orthogonal complement $\boldsymbol{S}^{\perp}$ of $\boldsymbol{S}$?

(c) What is the smallest possible size of a matrix A that has row space $\boldsymbol{S}$?

(d) What is the smallest possible size of a matrix B that has nullspace $\boldsymbol{S}^{\perp}$?

Solution

(a) If $\boldsymbol{S}$ is six-dimensional in $\mathbf{R}^9$, subspaces orthogonal to $\boldsymbol{S}$ can have dimensions $0, 1, 2, 3$.

(b) The complement $\boldsymbol{S}^{\perp}$ is the largest orthogonal subspace, with dimension 3.

(c) The smallest matrix A is 6 by 9 (its six rows will be a basis for $\boldsymbol{S}$).

(d) This is the same as question (c) !

If a new row 7 of B is a combination of the six rows of A, then B has the same row space as A. It also has the same nullspace. The special solutions $\boldsymbol{s}_1, \boldsymbol{s}_2, \boldsymbol{s}_3$ to $A\boldsymbol{x} = \mathbf{0}$. will be the same for $B\boldsymbol{x} = \mathbf{0}$. Elimination will change row 7 of B to all zeros.

4.1 B The equation $x - 3y - 4z = 0$ describes a plane $\boldsymbol{P}$ in $\mathbf{R}^3$ (actually a subspace).

(a) The plane $\boldsymbol{P}$ is the nullspace $\boldsymbol{N}(A)$ of what 1 by 3 matrix A? *Ans*: $A = [1 \; -3 \; -4]$.

(b) Find a basis $\boldsymbol{s}_1, \boldsymbol{s}_2$ of special solutions of $x - 3y - 4z = 0$ (these would be the columns of the nullspace matrix N). *Answer*: $\boldsymbol{s}_1 = (3, 1, 0)$ and $\boldsymbol{s}_2 = (4, 0, 1)$.

(c) Find a basis for the line $\boldsymbol{P}^{\perp}$ that is perpendicular to $\boldsymbol{P}$. *Answer*: $(1, -3, -4)$**!**

Problem Set 4.1

Questions 1–12 grow out of Figures 4.2 and 4.3 with four subspaces.

1 Construct any 2 by 3 matrix of rank one. Copy Figure 4.2 and put one vector in each subspace (and put two in the nullspace). Which vectors are orthogonal?

2 Redraw Figure 4.3 for a 3 by 2 matrix of rank $r = 2$. Which subspace is $\boldsymbol{Z}$ (zero vector only)? The nullspace part of any vector $\boldsymbol{x}$ in $\mathbf{R}^2$ is $\boldsymbol{x}_n =$ ____ .

3 Construct a matrix with the required property or say why that is impossible:

(a) Column space contains $\begin{bmatrix} 1 \\ 2 \\ -3 \end{bmatrix}$ and $\begin{bmatrix} 2 \\ -3 \\ 5 \end{bmatrix}$, nullspace contains $\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$

(b) Row space contains $\begin{bmatrix} 1 \\ 2 \\ -3 \end{bmatrix}$ and $\begin{bmatrix} 2 \\ -3 \\ 5 \end{bmatrix}$, nullspace contains $\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$

(c) $A\boldsymbol{x} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$ has a solution and $A^{\mathrm{T}} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$

(d) Every row is orthogonal to every column (A is not the zero matrix)

(e) Columns add up to a column of zeros, rows add to a row of 1's.

4 If $AB = 0$ then the columns of B are in the ____ of A. The rows of A are in the ____ of B. With $AB = 0$, why can't A and B be 3 by 3 matrices of rank 2?

5 (a) If $A\boldsymbol{x} = \boldsymbol{b}$ has a solution and $A^{\mathrm{T}}\boldsymbol{y} = \boldsymbol{0}$, *is* $(\boldsymbol{y}^{\mathrm{T}}\boldsymbol{x} = 0)$ *or* $(\boldsymbol{y}^{\mathrm{T}}\boldsymbol{b} = 0)$?

(b) If $A^{\mathrm{T}}\boldsymbol{y} = (1, 1, 1)$ has a solution and $A\boldsymbol{x} = \boldsymbol{0}$, then ____ .

6 This system of equations $A\boldsymbol{x} = \boldsymbol{b}$ has *no solution* (they lead to $0 = 1$):

$$\begin{aligned} x + 2y + 2z &= 5 \\ 2x + 2y + 3z &= 5 \\ 3x + 4y + 5z &= 9 \end{aligned}$$

Find numbers y_1, y_2, y_3 to multiply the equations so they add to $0 = 1$. You have found a vector $\boldsymbol{y}$ in which subspace? Its dot product $\boldsymbol{y}^{\mathrm{T}}\boldsymbol{b}$ is 1, so no solution $\boldsymbol{x}$.

7 Every system with no solution is like the one in Problem 6. There are numbers $y_1, \ldots, y_m$ that multiply the m equations so they add up to $0 = 1$. This is called **Fredholm's Alternative**:

Exactly one of these problems has a solution

$$A\boldsymbol{x} = \boldsymbol{b} \quad \textbf{OR} \quad A^{\mathrm{T}}\boldsymbol{y} = \boldsymbol{0} \quad \text{with} \quad \boldsymbol{y}^{\mathrm{T}}\boldsymbol{b} = 1.$$

If $\boldsymbol{b}$ is not in the column space of A, it is not orthogonal to the nullspace of A^{T}. Multiply the equations $x_1 - x_2 = 1$ and $x_2 - x_3 = 1$ and $x_1 - x_3 = 1$ by numbers y_1, y_2, y_3 chosen so that the equations add up to $0 = 1$.

8 In Figure 4.3, how do we know that $A\boldsymbol{x}_r$ is equal to $A\boldsymbol{x}$? How do we know that this vector is in the column space? If $A = \left[\begin{smallmatrix}1 & 1\\ 1 & 1\end{smallmatrix}\right]$ and $\boldsymbol{x} = \left[\begin{smallmatrix}1\\ 0\end{smallmatrix}\right]$ what is $\boldsymbol{x}_r$?

9 If $A^{\mathrm{T}}A\boldsymbol{x} = \mathbf{0}$ then $A\boldsymbol{x} = \mathbf{0}$. Reason: $A\boldsymbol{x}$ is in the nullspace of A^{T} and also in the _____ of A and those spaces are _____. *Conclusion*: *$A^{\mathrm{T}}A$ has the same nullspace as A. This key fact is repeated in the next section.*

10 Suppose A is a symmetric matrix ($A^{\mathrm{T}} = A$).

(a) Why is its column space perpendicular to its nullspace?

(b) If $A\boldsymbol{x} = \mathbf{0}$ and $A\boldsymbol{z} = 5\boldsymbol{z}$, which subspaces contain these "eigenvectors" $\boldsymbol{x}$ and $\boldsymbol{z}$? **Symmetric matrices have perpendicular eigenvectors $\boldsymbol{x}^{\mathrm{T}}\boldsymbol{z} = 0$.**

11 (Recommended) Draw Figure 4.2 to show each subspace correctly for

$$A = \begin{bmatrix} 1 & 2 \\ 3 & 6 \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} 1 & 0 \\ 3 & 0 \end{bmatrix}.$$

12 Find the pieces $\boldsymbol{x}_r$ and $\boldsymbol{x}_n$ and draw Figure 4.3 properly if

$$A = \begin{bmatrix} 1 & -1 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \quad \text{and} \quad \boldsymbol{x} = \begin{bmatrix} 2 \\ 0 \end{bmatrix}.$$

Questions 13–23 are about orthogonal subspaces.

13 Put bases for the subspaces $\boldsymbol{V}$ and $\boldsymbol{W}$ into the columns of matrices V and W. Explain why the test for orthogonal subspaces can be written $V^{\mathrm{T}}W$ = zero matrix. This matches $\boldsymbol{v}^{\mathrm{T}}\boldsymbol{w} = 0$ for orthogonal vectors.

14 The floor $\boldsymbol{V}$ and the wall $\boldsymbol{W}$ are not orthogonal subspaces, because they share a nonzero vector (along the line where they meet). No planes $\boldsymbol{V}$ and $\boldsymbol{W}$ in $\mathbf{R}^3$ can be orthogonal! Find a vector in the column spaces of both matrices:

$$A = \begin{bmatrix} 1 & 2 \\ 1 & 3 \\ 1 & 2 \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} 5 & 4 \\ 6 & 3 \\ 5 & 1 \end{bmatrix}$$

This will be a vector $A\boldsymbol{x}$ and also $B\widehat{\boldsymbol{x}}$. Think 3 by 4 with the matrix $[\,A \quad B\,]$.

15 Extend Problem 14 to a p-dimensional subspace $\boldsymbol{V}$ and a q-dimensional subspace $\boldsymbol{W}$ of $\mathbf{R}^n$. What inequality on $p + q$ guarantees that $\boldsymbol{V}$ intersects $\boldsymbol{W}$ in a nonzero vector? These subspaces cannot be orthogonal.

16 Prove that every $\boldsymbol{y}$ in $\boldsymbol{N}(A^{\mathrm{T}})$ is perpendicular to every $A\boldsymbol{x}$ in the column space, using the matrix shorthand of equation (2). Start from $A^{\mathrm{T}}\boldsymbol{y} = \mathbf{0}$.

17 If S is the subspace of $\mathbf{R}^3$ containing only the zero vector, what is $S^\perp$? If S is spanned by $(1,1,1)$, what is $S^\perp$? If S is spanned by $(1,1,1)$ and $(1,1,-1)$, what is a basis for $S^\perp$?

18 Suppose S only contains two vectors $(1,5,1)$ and $(2,2,2)$ (not a subspace). Then $S^\perp$ is the nullspace of the matrix $A =$ _____. $S^\perp$ is a subspace even if S is not.

19 Suppose $\boldsymbol{L}$ is a one-dimensional subspace (a line) in $\mathbf{R}^3$. Its orthogonal complement $\boldsymbol{L}^\perp$ is the _____ perpendicular to $\boldsymbol{L}$. Then $(\boldsymbol{L}^\perp)^\perp$ is a _____ perpendicular to $\boldsymbol{L}^\perp$. In fact $(\boldsymbol{L}^\perp)^\perp$ is the same as _____.

20 Suppose $\boldsymbol{V}$ is the whole space $\mathbf{R}^4$. Then $\boldsymbol{V}^\perp$ contains only the vector _____. Then $(\boldsymbol{V}^\perp)^\perp$ is _____. So $(\boldsymbol{V}^\perp)^\perp$ is the same as _____.

21 Suppose S is spanned by the vectors $(1,2,2,3)$ and $(1,3,3,2)$. Find two vectors that span $S^\perp$. This is the same as solving $A\boldsymbol{x} = \mathbf{0}$ for which A?

22 If $\boldsymbol{P}$ is the plane of vectors in $\mathbf{R}^4$ satisfying $x_1 + x_2 + x_3 + x_4 = 0$, write a basis for $\boldsymbol{P}^\perp$. Construct a matrix that has $\boldsymbol{P}$ as its nullspace.

23 If a subspace S is contained in a subspace $\boldsymbol{V}$, prove that $S^\perp$ contains $\boldsymbol{V}^\perp$.

Questions 24–30 are about perpendicular columns and rows.

24 Suppose an n by n matrix is invertible: $AA^{-1} = I$. Then the first column of A^{-1} is orthogonal to the space spanned by which rows of A?

25 Find $A^{\mathrm{T}}A$ if the columns of A are unit vectors, all mutually perpendicular.

26 Construct a 3 by 3 matrix A with no zero entries whose columns are mutually perpendicular. Compute $A^{\mathrm{T}}A$. Why is it a diagonal matrix?

27 The lines $3x+y=b_1$ and $6x+2y=b_2$ are _____. They are the same line if _____. In that case (b_1,b_2) is perpendicular to the vector _____. The nullspace of the matrix is the line $3x+y=$ _____. One particular vector in that nullspace is _____.

28 Why is each of these statements false?

(a) $(1,1,1)$ is perpendicular to $(1,1,-2)$ so the planes $x+y+z=0$ and $x+y-2z=0$ are orthogonal subspaces.

(b) The subspace spanned by $(1,1,0,0,0)$ and $(0,0,0,1,1)$ is the orthogonal complement of the subspace spanned by $(1,-1,0,0,0)$ and $(2,-2,3,4,-4)$.

(c) Two subspaces that meet only in the zero vector are orthogonal.

29 Find a matrix with $\boldsymbol{v} = (1,2,3)$ in the row space and column space. Find another matrix with $\boldsymbol{v}$ in the nullspace and column space. Which pairs of subspaces can $\boldsymbol{v}$ *not* be in?

Challenge Problems

30 Suppose A is 3 by 4 and B is 4 by 5 and $AB = 0$. So $\boldsymbol{N}(A)$ contains $\boldsymbol{C}(B)$. Prove from the dimensions of $\boldsymbol{N}(A)$ and $\boldsymbol{C}(B)$ that $\operatorname{rank}(A) + \operatorname{rank}(B) \leq 4$.

31 The command $N = \mathsf{null}(A)$ will produce a basis for the nullspace of A. Then the command $B = \mathsf{null}(N')$ will produce a basis for the _____ of A.

32 Suppose I give you four nonzero vectors $\boldsymbol{r}, \boldsymbol{n}, \boldsymbol{c}, \boldsymbol{l}$ in $\mathbf{R}^2$.

(a) What are the conditions for those to be bases for the four fundamental subspaces $C(A^{\mathrm{T}}), N(A), C(A), N(A^{\mathrm{T}})$ of a 2 by 2 matrix?

(b) What is one possible matrix A?

33 Suppose I give you eight vectors $\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{n}_1, \boldsymbol{n}_2, \boldsymbol{c}_1, \boldsymbol{c}_2, \boldsymbol{l}_1, \boldsymbol{l}_2$ in $\mathbf{R}^4$.

(a) What are the conditions for those pairs to be bases for the four fundamental subspaces of a 4 by 4 matrix?

(b) What is one possible matrix A?

4.2 Projections

1 The projection of a vector $\boldsymbol{b}$ onto the line through $\boldsymbol{a}$ is the closest point $\boldsymbol{p} = \boldsymbol{a}(\boldsymbol{a}^{\mathrm{T}}\boldsymbol{b}\,/\,\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a})$.

2 The error $\boldsymbol{e} = \boldsymbol{b} - \boldsymbol{p}$ is perpendicular to $\boldsymbol{a}$: Right triangle $\boldsymbol{b}\,\boldsymbol{p}\,\boldsymbol{e}$ has $||\boldsymbol{p}||^2 + ||\boldsymbol{e}||^2 = ||\boldsymbol{b}||^2$.

3 The **projection** of $\boldsymbol{b}$ onto a subspace $\boldsymbol{S}$ is the closest vector $\boldsymbol{p}$ in $\boldsymbol{S}$; $\boldsymbol{b} - \boldsymbol{p}$ is orthogonal to $\boldsymbol{S}$.

4 $A^{\mathrm{T}}A$ is invertible (and symmetric) only if A has independent columns: $\boldsymbol{N}(A^{\mathrm{T}}A) = \boldsymbol{N}(A)$.

5 Then the projection of $\boldsymbol{b}$ onto the column space of A is the vector $\boldsymbol{p} = A(A^{\mathrm{T}}A)^{-1}A^{\mathrm{T}}\boldsymbol{b}$.

6 The **projection matrix** onto $\boldsymbol{C}(A)$ is $\boxed{P = A(A^{\mathrm{T}}A)^{-1}A^{\mathrm{T}}.}$ It has $\boldsymbol{p} = P\boldsymbol{b}$ and $P^2 = P = P^{\mathrm{T}}$.

May we start this section with two questions? (In addition to that one.) The first question aims to show that projections are easy to visualize. The second question is about "projection matrices"—symmetric matrices with $P^2 = P$. *The projection of* $\boldsymbol{b}$ *is* $P\boldsymbol{b}$.

1 What are the projections of $\boldsymbol{b} = (2, 3, 4)$ onto the z axis and the xy plane?

2 What matrices P_1 and P_2 produce those projections onto a line and a plane?

When $\boldsymbol{b}$ is projected onto a line, ***its projection p is the part of b along that line***. If $\boldsymbol{b}$ is projected onto a plane, $\boldsymbol{p}$ is the part in that plane. ***The projection p is*** $P\boldsymbol{b}$.

The projection matrix P multiplies $\boldsymbol{b}$ to give $\boldsymbol{p}$. This section finds $\boldsymbol{p}$ and also P.

The projection onto the z axis we call $\boldsymbol{p}_1$. The second projection drops straight down to the xy plane. The picture in your mind should be Figure 4.5. Start with $\boldsymbol{b} = (2, 3, 4)$. The projection across gives $\boldsymbol{p}_1 = (0, 0, 4)$. The projection down gives $\boldsymbol{p}_2 = (2, 3, 0)$. Those are the parts of $\boldsymbol{b}$ along the z axis and in the xy plane.

The projection matrices P_1 and P_2 are 3 by 3. They multiply $\boldsymbol{b}$ with 3 components to produce $\boldsymbol{p}$ with 3 components. Projection onto a line comes from a rank one matrix. Projection onto a plane comes from a rank two matrix:

Projection matrix
Onto the z axis: $$P_1 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \mathbf{1} \end{bmatrix} \qquad \text{Onto the } xy \text{ plane:} \quad P_2 = \begin{bmatrix} \mathbf{1} & 0 & 0 \\ 0 & \mathbf{1} & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

P_1 picks out the z component of every vector. P_2 picks out the x and y components. To find the projections $\boldsymbol{p}_1$ and $\boldsymbol{p}_2$ of $\boldsymbol{b}$, multiply $\boldsymbol{b}$ by P_1 and P_2 (small $\boldsymbol{p}$ for the vector, capital P for the matrix that produces it):

$$\boldsymbol{p}_1 = P_1\boldsymbol{b} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \\ \boldsymbol{z} \end{bmatrix} \qquad \boldsymbol{p}_2 = P_2\boldsymbol{b} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} \boldsymbol{x} \\ \boldsymbol{y} \\ \mathbf{0} \end{bmatrix}.$$

In this case the projections p_1 and p_2 are perpendicular. The xy plane and the z axis are ***orthogonal subspaces***, like the floor of a room and the line between two walls.

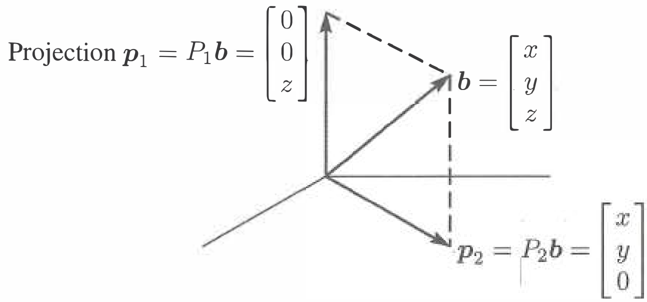


Figure 4.5: The projections $\boldsymbol{p}_1 = P_1\boldsymbol{b}$ and $\boldsymbol{p}_2 = P_2\boldsymbol{b}$ onto the z axis and the xy plane.

More than just orthogonal, the line and plane are orthogonal ***complements***. Their dimensions add to $1 + 2 = 3$. Every vector $\boldsymbol{b}$ in the whole space is the sum of its parts in the two subspaces. The projections $\boldsymbol{p}_1$ and $\boldsymbol{p}_2$ are exactly those two parts of $\boldsymbol{b}$:

$$\text{The vectors give } \boldsymbol{p}_1 + \boldsymbol{p}_2 = \boldsymbol{b}. \qquad \text{The matrices give } P_1 + P_2 = I. \tag{1}$$

This is perfect. Our goal is reached—for this example. We have the same goal for any line and any plane and any n-dimensional subspace. The object is to find the part $\boldsymbol{p}$ in each subspace, and the projection matrix P that produces that part $\boldsymbol{p} = P\boldsymbol{b}$. Every subspace of $\mathbf{R}^m$ has its own m by m projection matrix. To compute P, we absolutely need a good description of the subspace that it projects onto.

The best description of a subspace is a basis. We put the basis vectors into the columns of A. ***Now we are projecting onto the column space of A!*** Certainly the z axis is the column space of the 3 by 1 matrix A_1. The xy plane is the column space of A_2. That plane is *also* the column space of A_3 (a subspace has many bases). So $\boldsymbol{p}_2 = \boldsymbol{p}_3$ and $P_2 = P_3$.

$$A_1 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \quad \text{and} \quad A_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} \quad \text{and} \quad A_3 = \begin{bmatrix} 1 & 2 \\ 2 & 3 \\ 0 & 0 \end{bmatrix}.$$

Our problem is ***to project any b onto the column space of any m by n matrix***. Start with a line (dimension $n = 1$). The matrix A will have only one column. Call it $\boldsymbol{a}$.

Projection Onto a Line

A line goes through the origin in the direction of $\boldsymbol{a} = (a_1, \ldots, a_m)$. Along that line, we want the point $\boldsymbol{p}$ closest to $\boldsymbol{b} = (b_1, \ldots, b_m)$. The key to projection is orthogonality: ***The line from b to p is perpendicular to the vector a.*** This is the dotted line marked $\boldsymbol{e} = \boldsymbol{b} - \boldsymbol{p}$ for the error on the left side of Figure 4.6. We now compute $\boldsymbol{p}$ by algebra.

The projection $\boldsymbol{p}$ will be some multiple of $\boldsymbol{a}$. Call it $\boldsymbol{p} = \widehat{x}\boldsymbol{a}$ = "x hat" times $\boldsymbol{a}$. Computing this number $\widehat{x}$ will give the vector $\boldsymbol{p}$. Then from the formula for $\boldsymbol{p}$, we will read off the projection matrix P. These three steps will lead to all projection matrices: **find $\widehat{x}$, then find the vector p, then find the matrix P.**

The dotted line $\boldsymbol{b} - \boldsymbol{p}$ is the "error" $\boldsymbol{e} = \boldsymbol{b} - \widehat{x}\boldsymbol{a}$. It is perpendicular to $\boldsymbol{a}$—this will determine $\widehat{x}$. Use the fact that $\boldsymbol{b} - \widehat{x}\boldsymbol{a}$ **is perpendicular to** $\boldsymbol{a}$ when their dot product is zero:

Projecting $\boldsymbol{b}$ onto $\boldsymbol{a}$ with error $\boldsymbol{e} = \boldsymbol{b} - \widehat{x}\boldsymbol{a}$

$\boldsymbol{a} \cdot (\boldsymbol{b} - \widehat{x}\boldsymbol{a}) = 0$ or $\boldsymbol{a} \cdot \boldsymbol{b} - \widehat{x}\boldsymbol{a} \cdot \boldsymbol{a} = 0$

$$\widehat{x} = \frac{\boldsymbol{a} \cdot \boldsymbol{b}}{\boldsymbol{a} \cdot \boldsymbol{a}} = \frac{\boldsymbol{a}^{\mathrm{T}}\boldsymbol{b}}{\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a}}. \tag{2}$$

The multiplication $\boldsymbol{a}^{\mathrm{T}}\boldsymbol{b}$ is the same as $\boldsymbol{a} \cdot \boldsymbol{b}$. Using the transpose is better, because it applies also to matrices. Our formula $\widehat{x} = \boldsymbol{a}^{\mathrm{T}}\boldsymbol{b}/\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a}$ gives the projection $\boldsymbol{p} = \widehat{x}\boldsymbol{a}$.

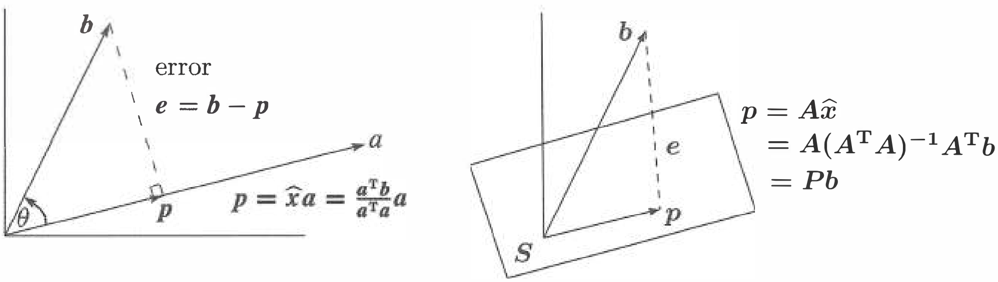


Figure 4.6: The projection $\boldsymbol{p}$ of $\boldsymbol{b}$ onto a line and onto $\boldsymbol{S}$ = column space of A.

The projection of b onto the line through a is the vector $\boldsymbol{p} = \widehat{x}\boldsymbol{a} = \dfrac{\boldsymbol{a}^{\mathrm{T}}\boldsymbol{b}}{\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a}}\boldsymbol{a}$.

Special case 1: If $\boldsymbol{b} = \boldsymbol{a}$ then $\widehat{x} = 1$. The projection of $\boldsymbol{a}$ onto $\boldsymbol{a}$ is itself. $P\boldsymbol{a} = \boldsymbol{a}$.

Special case 2: If $\boldsymbol{b}$ is perpendicular to $\boldsymbol{a}$ then $\boldsymbol{a}^{\mathrm{T}}\boldsymbol{b} = 0$. The projection is $\boldsymbol{p} = \boldsymbol{0}$.

Example 1 Project $\boldsymbol{b} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$ onto $\boldsymbol{a} = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}$ to find $\boldsymbol{p} = \widehat{x}\boldsymbol{a}$ in Figure 4.6.

Solution The number $\widehat{x}$ is the ratio of $\boldsymbol{a}^{\mathrm{T}}\boldsymbol{b} = 5$ to $\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a} = 9$. So the projection is $\boldsymbol{p} = \frac{5}{9}\boldsymbol{a}$.

The error vector between $\boldsymbol{b}$ and $\boldsymbol{p}$ is $\boldsymbol{e} = \boldsymbol{b} - \boldsymbol{p}$. Those vectors $\boldsymbol{p}$ and $\boldsymbol{e}$ will add to $\boldsymbol{b} = (\mathbf{1}, \mathbf{1}, \mathbf{1})$:

$$\boldsymbol{p} = \frac{5}{9}\boldsymbol{a} = \left(\frac{5}{9}, \frac{10}{9}, \frac{10}{9}\right) \quad \text{and} \quad \boldsymbol{e} = \boldsymbol{b} - \boldsymbol{p} = \left(\frac{4}{9}, -\frac{1}{9}, -\frac{1}{9}\right).$$

The error $\boldsymbol{e}$ should be perpendicular to $\boldsymbol{a} = (1, 2, 2)$ and it is: $\boldsymbol{e}^{\mathrm{T}}\boldsymbol{a} = \frac{4}{9} - \frac{2}{9} - \frac{2}{9} = 0$.

Look at the right triangle of $\boldsymbol{b}$, $\boldsymbol{p}$, and $\boldsymbol{e}$. The vector $\boldsymbol{b}$ is split into two parts—its component along the line is $\boldsymbol{p}$, its perpendicular part is $\boldsymbol{e}$. Those two sides $\boldsymbol{p}$ and $\boldsymbol{e}$ have length $||\boldsymbol{p}|| = ||\boldsymbol{b}|| \cos\theta$ and $||\boldsymbol{e}|| = ||\boldsymbol{b}|| \sin\theta$. Trigonometry matches the dot product:

$$\boldsymbol{p} = \frac{\boldsymbol{a}^{\mathrm{T}}\boldsymbol{b}}{\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a}}\boldsymbol{a} \quad \text{has length} \quad \boxed{||\boldsymbol{p}||} = \frac{||\boldsymbol{a}||\,||\boldsymbol{b}|| \cos\theta}{||\boldsymbol{a}||^2}||\boldsymbol{a}|| = \boxed{||\boldsymbol{b}|| \cos\theta.} \tag{3}$$

The dot product is a lot simpler than getting involved with $\cos\theta$ and the length of $\boldsymbol{b}$. The example has square roots in $\cos\theta = 5/3\sqrt{3}$ and $||\boldsymbol{b}|| = \sqrt{3}$. There are no square roots in the projection $\boldsymbol{p} = 5\boldsymbol{a}/9$. The good way to $5/9$ is $\boldsymbol{a}^{\mathrm{T}}\boldsymbol{b}/\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a}$.

Now comes the ***projection matrix***. In the formula for $\boldsymbol{p}$, what matrix is multiplying $\boldsymbol{b}$? You can see the matrix better if the number $\widehat{\boldsymbol{x}}$ is on the right side of $\boldsymbol{a}$:

Projection matrix P $\quad \boldsymbol{p} = \boldsymbol{a}\widehat{\boldsymbol{x}} = \boldsymbol{a}\dfrac{\boldsymbol{a}^{\mathrm{T}}\boldsymbol{b}}{\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a}} = P\boldsymbol{b}$ ***when the matrix is*** $P = \dfrac{\boldsymbol{a}\boldsymbol{a}^{\mathrm{T}}}{\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a}}$.

P is a column times a row! The column is $\boldsymbol{a}$, the row is $\boldsymbol{a}^{\mathrm{T}}$. Then divide by the number $\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a}$. The projection matrix P is m by m, but ***its rank is one***. We are projecting onto a one-dimensional subspace, the line through $\boldsymbol{a}$. *That line is the column space of P.*

Example 2 Find the projection matrix $P = \dfrac{\boldsymbol{a}\boldsymbol{a}^{\mathrm{T}}}{\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a}}$ onto the line through $\boldsymbol{a} = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}$.

Solution Multiply column $\boldsymbol{a}$ times row $\boldsymbol{a}^{\mathrm{T}}$ and divide by $\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a} = 9$:

$$\text{Projection matrix} \qquad P = \frac{\boldsymbol{a}\boldsymbol{a}^{\mathrm{T}}}{\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a}} = \frac{1}{9}\begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}\begin{bmatrix} 1 & 2 & 2 \end{bmatrix} = \frac{1}{9}\begin{bmatrix} 1 & 2 & 2 \\ 2 & 4 & 4 \\ 2 & 4 & 4 \end{bmatrix}.$$

This matrix projects *any* vector $\boldsymbol{b}$ onto $\boldsymbol{a}$. Check $\boldsymbol{p} = P\boldsymbol{b}$ for $\boldsymbol{b} = (1, 1, 1)$ in Example 1:

$$\boldsymbol{p} = P\boldsymbol{b} = \frac{1}{9}\begin{bmatrix} 1 & 2 & 2 \\ 2 & 4 & 4 \\ 2 & 4 & 4 \end{bmatrix}\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} = \frac{1}{9}\begin{bmatrix} 5 \\ 10 \\ 10 \end{bmatrix} \quad \text{which is correct.}$$

If the vector $\boldsymbol{a}$ is doubled, the matrix P stays the same! It still projects onto the same line. If the matrix is squared, P^2 equals P. ***Projecting a second time doesn't change anything***, **so $P^2 = P$**. The diagonal entries of P add up to $\frac{1}{9}(1 + 4 + 4) = 1$.

The matrix $I-P$ should be a projection too. It produces the other side $\boldsymbol{e}$ of the triangle—the perpendicular part of $\boldsymbol{b}$. Note that $(I-P)\boldsymbol{b}$ equals $\boldsymbol{b}-\boldsymbol{p}$ which is $\boldsymbol{e}$ in the left nullspace.

***When** P **projects onto one subspace**, $I-P$ **projects onto the perpendicular subspace**.* Here $I-P$ projects onto the plane perpendicular to $\boldsymbol{a}$.

Now we move beyond projection onto a line. Projecting onto an n-dimensional subspace of $\mathbf{R}^m$ takes more effort. The crucial formulas will be collected in equations (5)–(6)–(7). Basically you need to remember those three equations.

Projection Onto a Subspace

Start with n vectors $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_n$ in $\mathbf{R}^m$. Assume that these $\boldsymbol{a}$'s are linearly independent.

***Problem: Find the combination** $\boldsymbol{p} = \widehat{x}_1\boldsymbol{a}_1 + \cdots + \widehat{x}_n\boldsymbol{a}_n$ **closest to a given vector** $\boldsymbol{b}$.* We are projecting each $\boldsymbol{b}$ in $\mathbf{R}^m$ onto the subspace spanned by the $\boldsymbol{a}$'s.

With $n=1$ (one vector $\boldsymbol{a}_1$) this is projection onto a line. The line is the column space of A, which has just one column. In general the matrix A has n columns $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_n$.

The combinations in $\mathbf{R}^m$ are the vectors $A\boldsymbol{x}$ in the column space. We are looking for the particular combination $\boldsymbol{p} = A\widehat{\boldsymbol{x}}$ (***the projection***) that is closest to $\boldsymbol{b}$. The hat over $\widehat{\boldsymbol{x}}$ indicates the *best* choice $\widehat{\boldsymbol{x}}$, to give the closest vector in the column space. That choice is $\widehat{x} = \boldsymbol{a}^{\mathrm{T}}\boldsymbol{b}/\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a}$ when $n=1$. For $n>1$, the best $\widehat{\boldsymbol{x}} = (\widehat{x}_1, \ldots, \widehat{x}_n)$ is to be found now.

We compute projections onto n-dimensional subspaces in three steps as before: ***Find the vector*** $\widehat{\boldsymbol{x}}$, ***find the projection*** $\boldsymbol{p} = A\widehat{\boldsymbol{x}}$, ***find the projection matrix*** P.

The key is in the geometry! The dotted line in Figure 4.6 goes from $\boldsymbol{b}$ to the nearest point $A\widehat{\boldsymbol{x}}$ in the subspace. ***This error vector*** $\boldsymbol{b} - A\widehat{\boldsymbol{x}}$ ***is perpendicular to the subspace.*** The error $\boldsymbol{b} - A\widehat{\boldsymbol{x}}$ makes a right angle with all the vectors $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_n$ in the base. The n right angles give the n equations for $\widehat{\boldsymbol{x}}$:

$$\begin{array}{c} \boldsymbol{a}_1^{\mathrm{T}}(\boldsymbol{b} - A\widehat{\boldsymbol{x}}) = 0 \\ \vdots \\ \boldsymbol{a}_n^{\mathrm{T}}(\boldsymbol{b} - A\widehat{\boldsymbol{x}}) = 0 \end{array} \quad \text{or} \quad \begin{bmatrix} - \boldsymbol{a}_1^{\mathrm{T}} - \\ \vdots \\ - \boldsymbol{a}_n^{\mathrm{T}} - \end{bmatrix} \begin{bmatrix} \boldsymbol{b} - A\widehat{\boldsymbol{x}} \end{bmatrix} = \begin{bmatrix} \boldsymbol{0} \end{bmatrix}. \tag{4}$$

The matrix with those rows $\boldsymbol{a}_i^{\mathrm{T}}$ is A^{T}. The n equations are exactly $A^{\mathrm{T}}(\boldsymbol{b} - A\widehat{\boldsymbol{x}}) = \boldsymbol{0}$.

Rewrite $A^{\mathrm{T}}(\boldsymbol{b} - A\widehat{\boldsymbol{x}}) = \boldsymbol{0}$ in its famous form $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$. This is the equation for $\widehat{\boldsymbol{x}}$, and the coefficient matrix is $A^{\mathrm{T}}A$. Now we can find $\widehat{\boldsymbol{x}}$ and $\boldsymbol{p}$ and P, in that order.

The combination $p = \widehat{x}_1 a_1 + \cdots + \widehat{x}_n a_n = A\widehat{x}$ that is closest to b comes from $\widehat{x}$:

$$\textbf{Find } \widehat{x}\ (n \times 1) \qquad \boxed{A^{\mathrm{T}}(b - A\widehat{x}) = 0 \quad \text{or} \quad A^{\mathrm{T}}A\widehat{x} = A^{\mathrm{T}}b.} \tag{5}$$

This symmetric matrix $A^{\mathrm{T}}A$ is n by n. It is invertible if the a's are independent. The solution is $\widehat{x} = (A^{\mathrm{T}}A)^{-1}A^{\mathrm{T}}b$. The ***projection*** of b onto the subspace is p:

$$\textbf{Find } p\ (m \times 1) \qquad \boxed{p = A\widehat{x} = A(A^{\mathrm{T}}A)^{-1}A^{\mathrm{T}}b.} \tag{6}$$

The next formula picks out the ***projection matrix*** that is multiplying b in (6):

$$\textbf{Find } P\ (m \times m) \qquad \boxed{P = A(A^{\mathrm{T}}A)^{-1}A^{\mathrm{T}}.} \tag{7}$$

Compare with projection onto a line, when A has only one column: $A^{\mathrm{T}}A$ is $a^{\mathrm{T}}a$.

$$\textbf{For } n = 1 \qquad \boxed{\widehat{x} = \frac{a^{\mathrm{T}}b}{a^{\mathrm{T}}a}} \quad \textbf{and} \quad \boxed{p = a\frac{a^{\mathrm{T}}b}{a^{\mathrm{T}}a}} \quad \textbf{and} \quad \boxed{P = \frac{aa^{\mathrm{T}}}{a^{\mathrm{T}}a}.}$$

Those formulas are identical with (5) and (6) and (7). The number $a^{\mathrm{T}}a$ becomes the matrix $A^{\mathrm{T}}A$. When it is a number, we divide by it. When it is a matrix, we invert it. The new formulas contain $(A^{\mathrm{T}}A)^{-1}$ instead of $1/a^{\mathrm{T}}a$. The linear independence of the columns $a_1, \ldots, a_n$ will guarantee that this inverse matrix exists.

The key step was $A^{\mathrm{T}}(b - A\widehat{x}) = 0$. We used geometry ($e$ is orthogonal to each a). *Linear algebra gives this "normal equation" too*, in a very quick and beautiful way:

1. Our subspace is the column space of A.

2. The error vector $b - A\widehat{x}$ is perpendicular to that column space.

3. Therefore $b - A\widehat{x}$ is in the nullspace of A^{T}! This means $A^{\mathrm{T}}(b - A\widehat{x}) = 0$.

The left nullspace is important in projections. That nullspace of A^{T} contains the error vector $e = b - A\widehat{x}$. The vector b is being split into the projection p and the error $e = b - p$. Projection produces a right triangle with sides p, e, and b.

Example 3 If $A = \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \end{bmatrix}$ and $b = \begin{bmatrix} 6 \\ 0 \\ 0 \end{bmatrix}$ find $\widehat{x}$ and p and P.

Solution Compute the square matrix $A^{\mathrm{T}}A$ and also the vector $A^{\mathrm{T}}b$:

$$A^{\mathrm{T}}A = \begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 2 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \end{bmatrix} = \begin{bmatrix} 3 & 3 \\ 3 & 5 \end{bmatrix} \quad \text{and} \quad A^{\mathrm{T}}b = \begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 2 \end{bmatrix} \begin{bmatrix} 6 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 6 \\ 0 \end{bmatrix}.$$

Now solve the normal equation $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$ to find $\widehat{\boldsymbol{x}}$:

$$\begin{bmatrix} 3 & 3 \\ 3 & 5 \end{bmatrix} \begin{bmatrix} \widehat{x}_1 \\ \widehat{x}_2 \end{bmatrix} = \begin{bmatrix} 6 \\ 0 \end{bmatrix} \quad \text{gives} \quad \widehat{\boldsymbol{x}} = \begin{bmatrix} \widehat{x}_1 \\ \widehat{x}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{5} \\ \mathbf{-3} \end{bmatrix}. \tag{8}$$

The combination $\boldsymbol{p} = A\widehat{\boldsymbol{x}}$ is the projection of $\boldsymbol{b}$ onto the column space of A:

$$\boldsymbol{p} = 5 \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} - 3 \begin{bmatrix} 0 \\ 1 \\ 2 \end{bmatrix} = \begin{bmatrix} 5 \\ 2 \\ -1 \end{bmatrix}. \quad \text{The error is} \quad \boldsymbol{e} = \boldsymbol{b} - \boldsymbol{p} = \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}. \tag{9}$$

Two checks on the calculation. First, the error $\boldsymbol{e} = (1, -2, 1)$ is perpendicular to both columns $(1, 1, 1)$ and $(0, 1, 2)$. Second, the matrix P times $\boldsymbol{b} = (6, 0, 0)$ correctly gives $\boldsymbol{p} = (5, 2, -1)$. That solves the problem for one particular $\boldsymbol{b}$, as soon as we find P.

The projection matrix is $P = A(A^{\mathrm{T}}A)^{-1}A^{\mathrm{T}}$. The determinant of $A^{\mathrm{T}}A$ is $15 - 9 = 6$; then $(A^{\mathrm{T}}A)^{-1}$ is easy. Multiply A times $(A^{\mathrm{T}}A)^{-1}$ times A^{T} to reach P:

$$(A^{\mathrm{T}}A)^{-1} = \frac{1}{6} \begin{bmatrix} 5 & -3 \\ -3 & 3 \end{bmatrix} \quad \text{and} \quad P = \frac{1}{6} \begin{bmatrix} 5 & 2 & -1 \\ 2 & 2 & 2 \\ -1 & 2 & 5 \end{bmatrix}. \tag{10}$$

We must have $P^2 = P$, because a second projection doesn't change the first projection.

Warning The matrix $P = A(A^{\mathrm{T}}A)^{-1}A^{\mathrm{T}}$ is deceptive. You might try to split $(A^{\mathrm{T}}A)^{-1}$ into A^{-1} times $(A^{\mathrm{T}})^{-1}$. If you make that mistake, and substitute it into P, you will find $P = AA^{-1}(A^{\mathrm{T}})^{-1}A^{\mathrm{T}}$. Apparently everything cancels. This looks like $P = I$, the identity matrix. We want to say why this is wrong.

The matrix A is rectangular. It has no inverse matrix. We cannot split $(A^{\mathrm{T}}A)^{-1}$ into A^{-1} times $(A^{\mathrm{T}})^{-1}$ because there is no A^{-1} in the first place.

In our experience, a problem that involves a rectangular matrix almost always leads to $A^{\mathrm{T}}A$. When A has independent columns, $A^{\mathrm{T}}A$ is invertible. This fact is so crucial that we state it clearly and give a proof.

$A^{\mathrm{T}}A$ is invertible if and only if A has linearly independent columns.

Proof $A^{\mathrm{T}}A$ is a square matrix (n by n). For every matrix A, we will now show that $A^{\mathrm{T}}A$ ***has the same nullspace as*** A. When the columns of A are linearly independent, its nullspace contains only the zero vector. Then $A^{\mathrm{T}}A$, with this same nullspace, is invertible.

Let A be any matrix. If $\boldsymbol{x}$ is in its nullspace, then $A\boldsymbol{x} = \mathbf{0}$. Multiplying by A^{T} gives $A^{\mathrm{T}}A\boldsymbol{x} = \mathbf{0}$. So $\boldsymbol{x}$ is also in the nullspace of $A^{\mathrm{T}}A$.

Now start with the nullspace of $A^{\mathrm{T}}A$. **From** $A^{\mathrm{T}}A\boldsymbol{x} = \mathbf{0}$ **we must prove** $A\boldsymbol{x} = \mathbf{0}$. We can't multiply by $(A^{\mathrm{T}})^{-1}$, which generally doesn't exist. Just multiply by $\boldsymbol{x}^{\mathrm{T}}$:

$$(\boldsymbol{x}^{\mathrm{T}})A^{\mathrm{T}}A\boldsymbol{x} = 0 \quad \text{or} \quad (A\boldsymbol{x})^{\mathrm{T}}(A\boldsymbol{x}) = 0 \quad \text{or} \quad \|A\boldsymbol{x}\|^2 = 0. \tag{11}$$

We have shown: If $A^{\mathrm{T}}A\boldsymbol{x} = \mathbf{0}$ then $A\boldsymbol{x}$ has length zero. Therefore $A\boldsymbol{x} = \mathbf{0}$. Every vector $\boldsymbol{x}$ in one nullspace is in the other nullspace. If $A^{\mathrm{T}}A$ has dependent columns, so has A. If $A^{\mathrm{T}}A$ has independent columns, so has A. This is the good case: $A^{\mathrm{T}}A$ is invertible.

When A has independent columns, $A^{\mathrm{T}}A$ is square, symmetric, and invertible.

To repeat for emphasis: $A^{\mathrm{T}}A$ is (n by m) times (m by n). Then $A^{\mathrm{T}}A$ is square (n by n). It is symmetric, because its transpose is $(A^{\mathrm{T}}A)^{\mathrm{T}} = A^{\mathrm{T}}(A^{\mathrm{T}})^{\mathrm{T}}$ which equals $A^{\mathrm{T}}A$. We just proved that $A^{\mathrm{T}}A$ is invertible—provided A has independent columns. Watch the difference between dependent and independent columns:

$$\underset{A^{\mathrm{T}}}{\begin{bmatrix} 1 & 1 & 0 \\ 2 & 2 & 0 \end{bmatrix}} \underset{\text{dependent}}{\overset{A}{\begin{bmatrix} 1 & 2 \\ 1 & 2 \\ 0 & 0 \end{bmatrix}}} = \underset{\text{singular}}{\overset{A^{\mathrm{T}}A}{\begin{bmatrix} 2 & 4 \\ 4 & 8 \end{bmatrix}}} \qquad \underset{A^{\mathrm{T}}}{\begin{bmatrix} 1 & 1 & 0 \\ 2 & 2 & 1 \end{bmatrix}} \underset{\text{indep.}}{\overset{A}{\begin{bmatrix} 1 & 2 \\ 1 & 2 \\ 0 & 1 \end{bmatrix}}} = \underset{\text{invertible}}{\overset{A^{\mathrm{T}}A}{\begin{bmatrix} 2 & 4 \\ 4 & 9 \end{bmatrix}}}$$

Very brief summary To find the projection $\boldsymbol{p} = \widehat{x}_1\boldsymbol{a}_1 + \cdots + \widehat{x}_n\boldsymbol{a}_n$, solve $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$. This gives $\widehat{\boldsymbol{x}}$. The projection is $\boldsymbol{p} = A\widehat{\boldsymbol{x}}$ and the error is $\boldsymbol{e} = \boldsymbol{b} - \boldsymbol{p} = \boldsymbol{b} - A\widehat{\boldsymbol{x}}$. The projection matrix $P = A(A^{\mathrm{T}}A)^{-1}A^{\mathrm{T}}$ gives $\boldsymbol{p} = P\boldsymbol{b}$.

This matrix satisfies $P^2 = P$. *The distance from b to the subspace $C(A)$ is $\|e\|$.*

■ REVIEW OF THE KEY IDEAS ■

1. The projection of $\boldsymbol{b}$ onto the line through $\boldsymbol{a}$ is $\boldsymbol{p} = \boldsymbol{a}\widehat{\boldsymbol{x}} = \boldsymbol{a}(\boldsymbol{a}^{\mathrm{T}}\boldsymbol{b}/\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a})$.

2. The rank one projection matrix $P = \boldsymbol{a}\boldsymbol{a}^{\mathrm{T}}/\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a}$ multiplies $\boldsymbol{b}$ to produce $\boldsymbol{p}$.

3. Projecting $\boldsymbol{b}$ onto a subspace leaves $\boldsymbol{e} = \boldsymbol{b} - \boldsymbol{p}$ perpendicular to the subspace.

4. When A has full rank n, the equation $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$ leads to $\widehat{\boldsymbol{x}}$ and $\boldsymbol{p} = A\widehat{\boldsymbol{x}}$.

5. The projection matrix $P = A(A^{\mathrm{T}}A)^{-1}A^{\mathrm{T}}$ has $P^{\mathrm{T}} = P$ and $P^2 = P$ and $P\boldsymbol{b} = \boldsymbol{p}$.

■ WORKED EXAMPLES ■

4.2 A Project the vector $\boldsymbol{b} = (3, 4, 4)$ onto the line through $\boldsymbol{a} = (2, 2, 1)$ and then onto the plane that also contains $\boldsymbol{a}^* = (1, 0, 0)$. Check that the first error vector $\boldsymbol{b} - \boldsymbol{p}$ is perpendicular to $\boldsymbol{a}$, and the second error vector $\boldsymbol{e}^* = \boldsymbol{b} - \boldsymbol{p}^*$ is also perpendicular to $\boldsymbol{a}^*$.

Find the 3 by 3 projection matrix P onto that plane of $\boldsymbol{a}$ and $\boldsymbol{a}^*$. Find a vector whose *projection onto the plane is the zero vector*. Why is it exactly the error $\boldsymbol{e}^*$?

Solution The projection of $\boldsymbol{b} = (3,4,4)$ onto the line through $\boldsymbol{a} = (2,2,1)$ is $\boldsymbol{p} = 2\boldsymbol{a}$:

Onto a line $$\boldsymbol{p} = \frac{\boldsymbol{a}^{\mathrm{T}}\boldsymbol{b}}{\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a}}\boldsymbol{a} = \frac{18}{9}(2,2,1) = (4,4,2) = 2\boldsymbol{a}.$$

The error vector $\boldsymbol{e} = \boldsymbol{b} - \boldsymbol{p} = (-1,0,2)$ is perpendicular to $\boldsymbol{a} = (2,2,1)$. So $\boldsymbol{p}$ is correct.

The plane of $\boldsymbol{a} = (2,2,1)$ and $\boldsymbol{a}^* = (1,0,0)$ is the column space of $A = [\boldsymbol{a}\ \boldsymbol{a}^*]$:

$$A = \begin{bmatrix} 2 & 1 \\ 2 & 0 \\ 1 & 0 \end{bmatrix} \quad A^{\mathrm{T}}A = \begin{bmatrix} 9 & 2 \\ 2 & 1 \end{bmatrix} \quad (A^{\mathrm{T}}A)^{-1} = \frac{1}{5}\begin{bmatrix} 1 & -2 \\ -2 & 9 \end{bmatrix} \quad P = \begin{bmatrix} 1 & 0 & 0 \\ 0 & .8 & .4 \\ 0 & .4 & .2 \end{bmatrix}$$

Now $\boldsymbol{p}^* = P\boldsymbol{b} = (3, 4.8, 2.4)$. The error $\boldsymbol{e}^* = \boldsymbol{b} - \boldsymbol{p}^* = (0, -.8, 1.6)$ is perpendicular to $\boldsymbol{a}$ and $\boldsymbol{a}^*$. This $\boldsymbol{e}^*$ is in the nullspace of P and *its projection is zero*! Note $P^2 = P = P^{\mathrm{T}}$.

4.2 B Suppose your pulse is measured at $x = 70$ beats per minute, then at $x = 80$, then at $x = 120$. Those three equations $Ax = \boldsymbol{b}$ in one unknown have $A^{\mathrm{T}} = [1\ 1\ 1]$ and $\boldsymbol{b} = (70, 80, 120)$. ***The best $\widehat{x}$ is the _____ of* 70, 80, 120**. Use calculus and projection:

1. Minimize $E = (x-70)^2 + (x-80)^2 + (x-120)^2$ by solving $dE/dx = 0$.
2. Project $\boldsymbol{b} = (70, 80, 120)$ onto $\boldsymbol{a} = (1,1,1)$ to find $\widehat{x} = \boldsymbol{a}^{\mathrm{T}}\boldsymbol{b}/\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a}$.

Solution The closest horizontal line to the heights $70, 80, 120$ is the *average* $\widehat{x} = 90$:

$$\frac{dE}{dx} = 2(x-70) + 2(x-80) + 2(x-120) = 0 \quad \text{gives} \quad \widehat{x} = \frac{70+80+120}{3} = 90.$$

Also by projection : $$\widehat{x} = \frac{\boldsymbol{a}^{\mathrm{T}}\boldsymbol{b}}{\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a}} = \frac{(1,1,1)^{\mathrm{T}}(70,80,120)}{(1,1,1)^{\mathrm{T}}(1,1,1)} = \frac{70+80+120}{3} = 90.$$

In *recursive* least squares, a fourth measurement 130 changes the average $\widehat{x}_{\text{old}} = 90$ to $\widehat{x}_{\text{new}} = 100$. Verify the *update formula* $\widehat{x}_{\text{new}} = \widehat{x}_{\text{old}} + \frac{1}{4}(130 - \widehat{x}_{\text{old}})$. When a new measurement arrives, we don't have to average all the old measurements again!

Problem Set 4.2

Questions 1–9 ask for projections p onto lines. Also errors $e = b - p$ and matrices P.

1 Project the vector b onto the line through a. Check that e is perpendicular to a:

$$\text{(a)}\ \ b = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix} \ \text{ and } \ a = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \qquad \text{(b)}\ \ b = \begin{bmatrix} 1 \\ 3 \\ 1 \end{bmatrix} \ \text{ and } \ a = \begin{bmatrix} -1 \\ -3 \\ -1 \end{bmatrix}.$$

2 *Draw* the projection of b onto a and also compute it from $p = \widehat{x}a$:

$$\text{(a)}\ \ b = \begin{bmatrix} \cos\theta \\ \sin\theta \end{bmatrix} \quad \text{and} \quad a = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \text{(b)}\quad b = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad \text{and} \quad a = \begin{bmatrix} 1 \\ -1 \end{bmatrix}.$$

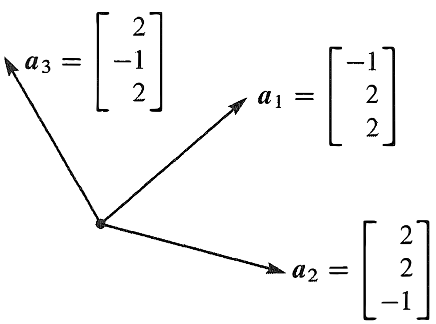
3 In Problem 1, find the projection matrix $P = aa^{\mathrm{T}}/a^{\mathrm{T}}a$ onto the line through each vector a. Verify in both cases that $P^2 = P$. Multiply Pb in each case to compute the projection p.

4 Construct the projection matrices P_1 and P_2 onto the lines through the a's in Problem 2. Is it true that $(P_1 + P_2)^2 = P_1 + P_2$? This *would* be true if $P_1 P_2 = 0$.

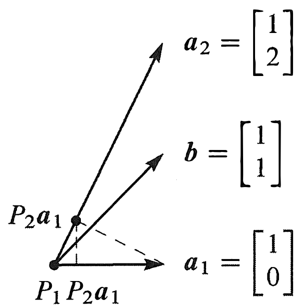
5 Compute the projection matrices $aa^{\mathrm{T}}/a^{\mathrm{T}}a$ onto the lines through $a_1 = (-1, 2, 2)$ and $a_2 = (2, 2, -1)$. Multiply those projection matrices and explain why their product $P_1 P_2$ is what it is.

6 Project $b = (1, 0, 0)$ onto the lines through a_1 and a_2 in Problem 5 and also onto $a_3 = (2, -1, 2)$. Add up the three projections $p_1 + p_2 + p_3$.

7 Continuing Problems 5–6, find the projection matrix P_3 onto $a_3 = (2, -1, 2)$. Verify that $P_1 + P_2 + P_3 = I$. This is because the basis a_1, a_2, a_3 is orthogonal!



Questions 5–6–7: orthogonal



Questions 8–9–10: not orthogonal

8 Project the vector $b = (1, 1)$ onto the lines through $a_1 = (1, 0)$ and $a_2 = (1, 2)$. Draw the projections p_1 and p_2 and add $p_1 + p_2$. The projections do not add to b because the a's are not orthogonal.

9 In Problem 8, the projection of b onto the *plane* of a_1 and a_2 will equal b. Find $P = A(A^{\mathrm{T}}A)^{-1}A^{\mathrm{T}}$ for $A = \begin{bmatrix} a_1 & a_2 \end{bmatrix} = \left[\begin{smallmatrix} 1 & 1 \\ 0 & 2 \end{smallmatrix}\right] =$ invertible matrix.

10 Project $a_1 = (1, 0)$ onto $a_2 = (1, 2)$. Then project the result back onto a_1. Draw these projections and multiply the projection matrices $P_1 P_2$: Is this a projection?

Questions 11–20 ask for projections, and projection matrices, onto subspaces.

11 Project $\boldsymbol{b}$ onto the column space of A by solving $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$ and $\boldsymbol{p} = A\widehat{\boldsymbol{x}}$:

$$\text{(a)}\quad A = \begin{bmatrix} 1 & 1 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} \quad \text{and} \quad \boldsymbol{b} = \begin{bmatrix} 2 \\ 3 \\ 4 \end{bmatrix} \qquad \text{(b)}\quad A = \begin{bmatrix} 1 & 1 \\ 1 & 1 \\ 0 & 1 \end{bmatrix} \quad \text{and} \quad \boldsymbol{b} = \begin{bmatrix} 4 \\ 4 \\ 6 \end{bmatrix}.$$

Find $\boldsymbol{e} = \boldsymbol{b} - \boldsymbol{p}$. It should be perpendicular to the columns of A.

12 Compute the projection matrices P_1 and P_2 onto the column spaces in Problem 11. Verify that $P_1\boldsymbol{b}$ gives the first projection $\boldsymbol{p}_1$. Also verify $P_2^2 = P_2$.

13 (Quick and Recommended) Suppose A is the 4 by 4 identity matrix with its last column removed. A is 4 by 3. Project $\boldsymbol{b} = (1, 2, 3, 4)$ onto the column space of A. What shape is the projection matrix P and what is P?

14 Suppose $\boldsymbol{b}$ equals 2 times the first column of A. What is the projection of $\boldsymbol{b}$ onto the column space of A? Is $P = I$ for sure in this case? Compute $\boldsymbol{p}$ and P when $\boldsymbol{b} = (0, 2, 4)$ and the columns of A are $(0, 1, 2)$ and $(1, 2, 0)$.

15 If A is doubled, then $P = 2A(4A^{\mathrm{T}}A)^{-1}2A^{\mathrm{T}}$. This is the same as $A(A^{\mathrm{T}}A)^{-1}A^{\mathrm{T}}$. The column space of $2A$ is the same as _____ . Is $\widehat{\boldsymbol{x}}$ the same for A and $2A$?

16 What linear combination of $(1, 2, -1)$ and $(1, 0, 1)$ is closest to $\boldsymbol{b} = (2, 1, 1)$?

17 (*Important*) If $P^2 = P$ show that $(I - P)^2 = I - P$. When P projects onto the column space of A, $I - P$ projects onto the _____ .

18 (a) If P is the 2 by 2 projection matrix onto the line through $(1, 1)$, then $I - P$ is the projection matrix onto _____ .

(b) If P is the 3 by 3 projection matrix onto the line through $(1, 1, 1)$, then $I - P$ is the projection matrix onto _____ .

19 To find the projection matrix onto the plane $x - y - 2z = 0$, choose two vectors in that plane and make them the columns of A. The plane will be the column space of A! Then compute $P = A(A^{\mathrm{T}}A)^{-1}A^{\mathrm{T}}$.

20 To find the projection matrix P onto the same plane $x - y - 2z = 0$, write down a vector $\boldsymbol{e}$ that is perpendicular to that plane. Compute the projection $Q = \boldsymbol{e}\boldsymbol{e}^{\mathrm{T}}/\boldsymbol{e}^{\mathrm{T}}\boldsymbol{e}$ and then $P = I - Q$.

Questions 21–26 show that projection matrices satisfy $\boldsymbol{P^2 = P}$ and $\boldsymbol{P^{\mathrm{T}} = P}$.

21 Multiply the matrix $P = A(A^{\mathrm{T}}A)^{-1}A^{\mathrm{T}}$ by itself. Cancel to prove that $P^2 = P$. Explain why $P(P\boldsymbol{b})$ always equals $P\boldsymbol{b}$: The vector $P\boldsymbol{b}$ is in the column space of A so its projection onto that column space is _____ .

22 Prove that $P = A(A^{\mathrm{T}}A)^{-1}A^{\mathrm{T}}$ is symmetric by computing P^{T}. Remember that the inverse of a symmetric matrix is symmetric.

23 If A is square and invertible, the warning against splitting $(A^{\mathrm{T}}A)^{-1}$ does not apply. It is true that $AA^{-1}(A^{\mathrm{T}})^{-1}A^{\mathrm{T}} = I$. *When A is invertible, why is $P = I$?* ***What is the error*** e?

24 The nullspace of A^{T} is _____ to the column space $\boldsymbol{C}(A)$. So if $A^{\mathrm{T}}\boldsymbol{b} = \mathbf{0}$, the projection of $\boldsymbol{b}$ onto $\boldsymbol{C}(A)$ should be $\boldsymbol{p} =$ _____. Check that $P = A(A^{\mathrm{T}}A)^{-1}A^{\mathrm{T}}$ gives this answer.

25 The projection matrix P onto an n-dimensional subspace of $\mathbf{R}^m$ has rank $r = n$. ***Reason:*** The projections $P\boldsymbol{b}$ fill the subspace S. So S is the _____ of P.

26 If an m by m matrix has $A^2 = A$ and its rank is m, prove that $A = I$.

27 The important fact that ends the section is this: ***If*** $\boldsymbol{A^{\mathrm{T}}Ax} = \mathbf{0}$ ***then*** $\boldsymbol{Ax} = \mathbf{0}$. *New Proof*: The vector $A\boldsymbol{x}$ is in the nullspace of _____. $A\boldsymbol{x}$ is always in the column space of _____. To be in both of those perpendicular spaces, $A\boldsymbol{x}$ must be zero.

28 Use $P^{\mathrm{T}} = P$ and $P^2 = P$ to prove that the length squared of column 2 always equals the diagonal entry P_{22}. This number is $\frac{2}{6} = \frac{4}{36} + \frac{4}{36} + \frac{4}{36}$ for

$$P = \frac{1}{6}\begin{bmatrix} 5 & 2 & -1 \\ 2 & 2 & 2 \\ -1 & 2 & 5 \end{bmatrix}.$$

29 If B has rank m (full row rank, independent rows) show that BB^{T} is invertible.

Challenge Problems

30 (a) Find the projection matrix P_C onto the column space of A (after looking closely at the matrix!)

$$A = \begin{bmatrix} 3 & 6 & 6 \\ 4 & 8 & 8 \end{bmatrix}$$

(b) Find the 3 by 3 projection matrix P_R onto the row space of A. Multiply $B = P_C A P_R$. Your answer B should be a little surprising—can you explain it?

31 In $\mathbf{R}^m$, suppose I give you $\boldsymbol{b}$ and also a combination $\boldsymbol{p}$ of $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_n$. How would you test to see if $\boldsymbol{p}$ is the projection of $\boldsymbol{b}$ onto the subspace spanned by the $\boldsymbol{a}$'s?

32 Suppose P_1 is the projection matrix onto the 1-dimensional subspace spanned by the first column of A. Suppose P_2 is the projection matrix onto the 2-dimensional column space of A. After thinking a little, compute the product P_2P_1.

$$A = \begin{bmatrix} 1 & 0 \\ 2 & 1 \\ 0 & 1 \end{bmatrix}.$$

33 Suppose you know the average $\widehat{x}_{\text{old}}$ of $b_1, b_2, \ldots, b_{999}$. When b_{1000} arrives, check that the new average is a combination of $\widehat{x}_{\text{old}}$ and the mismatch $b_{1000} - \widehat{x}_{\text{old}}$:

$$\widehat{\boldsymbol{x}}_{\textbf{new}} = \frac{b_1 + \cdots + b_{1000}}{1000} = \frac{b_1 + \cdots + b_{999}}{999} + \frac{1}{1000}\left(b_{1000} - \frac{b_1 + \cdots + b_{999}}{999}\right).$$

This is a "**Kalman filter**" $\widehat{x}_{\text{new}} = \widehat{x}_{\text{old}} + \frac{1}{1000}\left(b_{1000} - \widehat{x}_{\text{old}}\right)$ with gain matrix $\frac{1}{1000}$. The last page of the book extends the Kalman filter to matrix updates.

34 (2017) Suppose P_1 and P_2 are projection matrices ($P_i^2 = P_i = P_i^{\mathrm{T}}$). Prove this fact:

$$P_1 P_2 \text{ is a projection matrix if and only if } P_1 P_2 = P_2 P_1.$$

4.3 Least Squares Approximations

1 Solving $\boxed{A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}}$ gives the projection $\boldsymbol{p} = A\widehat{\boldsymbol{x}}$ of $\boldsymbol{b}$ onto the column space of A.

2 When $A\boldsymbol{x} = \boldsymbol{b}$ has no solution, $\widehat{\boldsymbol{x}}$ is the "least-squares solution": $||\boldsymbol{b} - A\widehat{\boldsymbol{x}}||^2 =$ minimum.

3 Setting partial derivatives of $E = ||A\boldsymbol{x} - \boldsymbol{b}||^2$ to zero $\left(\frac{\partial E}{\partial x_i} = 0\right)$ also produces $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$.

4 To fit points $(t_1, b_1), \ldots, (t_m, b_m)$ by a straight line, A has columns $(1, \ldots, 1)$ and $(t_1, \ldots, t_m)$.

5 In that case $A^{\mathrm{T}}A$ is the 2 by 2 matrix $\begin{bmatrix} m & \Sigma\, t_i \\ \Sigma\, t_i & \Sigma\, t_i^2 \end{bmatrix}$ and $A^{\mathrm{T}}\boldsymbol{b}$ is the vector $\begin{bmatrix} \Sigma\, b_i \\ \Sigma\, t_i b_i \end{bmatrix}$.

It often happens that $A\boldsymbol{x} = \boldsymbol{b}$ has no solution. The usual reason is: *too many equations*. The matrix A has more rows than columns. There are more equations than unknowns (m is greater than n). The n columns span a small part of m-dimensional space. Unless all measurements are perfect, $\boldsymbol{b}$ is outside that column space of A. Elimination reaches an impossible equation and stops. But we can't stop just because measurements include noise!

To repeat: We cannot always get the error $\boldsymbol{e} = \boldsymbol{b} - A\boldsymbol{x}$ down to zero. When $\boldsymbol{e}$ is zero, $\boldsymbol{x}$ is an exact solution to $A\boldsymbol{x} = \boldsymbol{b}$. *When the length of* $\boldsymbol{e}$ *is as small as possible,* $\widehat{\boldsymbol{x}}$ *is a least squares solution.* Our goal in this section is to compute $\widehat{\boldsymbol{x}}$ and use it. These are real problems and they need an answer.

The previous section emphasized $\boldsymbol{p}$ (the projection). This section emphasizes $\widehat{\boldsymbol{x}}$ (the least squares solution). They are connected by $\boldsymbol{p} = A\widehat{\boldsymbol{x}}$. The fundamental equation is still $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$. Here is a short unofficial way to reach this "*normal equation*":

When $A\boldsymbol{x} = \boldsymbol{b}$ has no solution, multiply by A^{T} and solve $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$.

Example 1 A crucial application of least squares is fitting a straight line to m points. Start with three points: *Find the closest line to the points* $(0, 6)$, $(1, 0)$, *and* $(2, 0)$.

No straight line $b = C + Dt$ goes through those three points. We are asking for two numbers C and D that satisfy three equations: $n = 2$ and $m = 3$. Here are the three equations at $t = 0, 1, 2$ to match the given values $b = 6, 0, 0$:

$\boldsymbol{t = 0}$	The first point is on the line $b = C + Dt$ if	$C + D \cdot 0 = 6$
$\boldsymbol{t = 1}$	The second point is on the line $b = C + Dt$ if	$C + D \cdot 1 = 0$
$\boldsymbol{t = 2}$	The third point is on the line $b = C + Dt$ if	$C + D \cdot 2 = 0.$

This 3 by 2 system has *no solution*: $\boldsymbol{b} = (6,0,0)$ is not a combination of the columns $(1,1,1)$ and $(0,1,2)$. Read off A, $\boldsymbol{x}$, and $\boldsymbol{b}$ from those equations:

$$A = \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \end{bmatrix} \quad \boldsymbol{x} = \begin{bmatrix} C \\ D \end{bmatrix} \quad \boldsymbol{b} = \begin{bmatrix} 6 \\ 0 \\ 0 \end{bmatrix} \quad A\boldsymbol{x} = \boldsymbol{b} \text{ is } \textit{not} \text{ solvable.}$$

The same numbers were in Example 3 in the last section. We computed $\widehat{\boldsymbol{x}} = (5, -3)$. **Those numbers are the best C and D, so $5 - 3t$ will be the best line for the 3 points.** We must connect projections to least squares, by explaining why $A^{\mathrm{T}} A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$.

In practical problems, there could easily be $m = 100$ points instead of $m = 3$. They don't exactly match any straight line $C + Dt$. Our numbers $6,0,0$ exaggerate the error so you can see e_1, e_2, and e_3 in Figure 4.6.

Minimizing the Error

How do we make the error $\boldsymbol{e} = \boldsymbol{b} - A\boldsymbol{x}$ as small as possible? This is an important question with a beautiful answer. The best $\boldsymbol{x}$ (called $\widehat{\boldsymbol{x}}$) can be found by geometry (the error $\boldsymbol{e}$ meets the column space of A at 90°) and by algebra: $A^{\mathrm{T}} A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$. Calculus gives the same $\widehat{\boldsymbol{x}}$: the derivative of the error $||A\boldsymbol{x} - \boldsymbol{b}||^2$ is zero at $\widehat{\boldsymbol{x}}$.

By geometry Every $A\boldsymbol{x}$ lies in the plane of the columns $(1,1,1)$ and $(0,1,2)$. In that plane, we look for the point closest to $\boldsymbol{b}$. *The nearest point is the projection* $\boldsymbol{p}$.

The best choice for $A\widehat{\boldsymbol{x}}$ is $\boldsymbol{p}$. The smallest possible error is $\boldsymbol{e} = \boldsymbol{b} - \boldsymbol{p}$, perpendicular to the columns. *The three points at heights* (p_1, p_2, p_3) *do lie on a line*, because $\boldsymbol{p}$ is in the column space of A. In fitting a straight line, $\widehat{\boldsymbol{x}}$ is the best choice for (C, D).

By algebra Every vector $\boldsymbol{b}$ splits into two parts. The part in the column space is $\boldsymbol{p}$. The perpendicular part is $\boldsymbol{e}$. There is an equation we cannot solve ($A\boldsymbol{x} = \boldsymbol{b}$). There is an equation $A\widehat{\boldsymbol{x}} = \boldsymbol{p}$ we can and do solve (by removing $\boldsymbol{e}$ and solving $A^{\mathrm{T}} A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$):

$$A\boldsymbol{x} = \boldsymbol{b} = \boldsymbol{p} + \boldsymbol{e} \quad \text{is impossible} \qquad A\widehat{\boldsymbol{x}} = \boldsymbol{p} \quad \text{is solvable} \qquad \widehat{\boldsymbol{x}} \text{ is } (A^{\mathrm{T}}A)^{-1}A^{\mathrm{T}}\boldsymbol{b}. \tag{1}$$

The solution to $A\widehat{\boldsymbol{x}} = \boldsymbol{p}$ leaves the least possible error (which is $\boldsymbol{e}$):

Squared length for any $\boldsymbol{x}$ $$||A\boldsymbol{x} - \boldsymbol{b}||^2 = ||A\boldsymbol{x} - \boldsymbol{p}||^2 + ||\boldsymbol{e}||^2. \tag{2}$$

This is the law $c^2 = a^2 + b^2$ for a right triangle. The vector $A\boldsymbol{x} - \boldsymbol{p}$ in the column space is perpendicular to $\boldsymbol{e}$ in the left nullspace. We reduce $A\boldsymbol{x} - \boldsymbol{p}$ to **zero** by choosing $\boldsymbol{x} = \widehat{\boldsymbol{x}}$. That leaves the smallest possible error $\boldsymbol{e} = (e_1, e_2, e_3)$ which we can't reduce.

Notice what "smallest" means. The *squared length* of $A\boldsymbol{x} - \boldsymbol{b}$ is minimized:

The least squares solution $\widehat{\boldsymbol{x}}$ makes $E = \|\|A\boldsymbol{x} - \boldsymbol{b}\|\|^2$ as small as possible.

Figure 4.6a shows the closest line. It misses by distances $e_1, e_2, e_3 = 1, -2, 1$. *Those are vertical distances*. The least squares line minimizes $E = e_1^2 + e_2^2 + e_3^2$.

Figure 4.6b shows the same problem in 3-dimensional space ($\boldsymbol{b}\,\boldsymbol{p}\,\boldsymbol{e}$ space). The vector $\boldsymbol{b}$ is not in the column space of A. That is why we could not solve $A\boldsymbol{x} = \boldsymbol{b}$. No line goes through the three points. The smallest possible error is the perpendicular vector $\boldsymbol{e}$. This is $\boldsymbol{e} = \boldsymbol{b} - A\widehat{\boldsymbol{x}}$, the vector of errors $(1, -2, 1)$ in the three equations. Those are the distances from the best line. Behind both figures is the fundamental equation $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$.

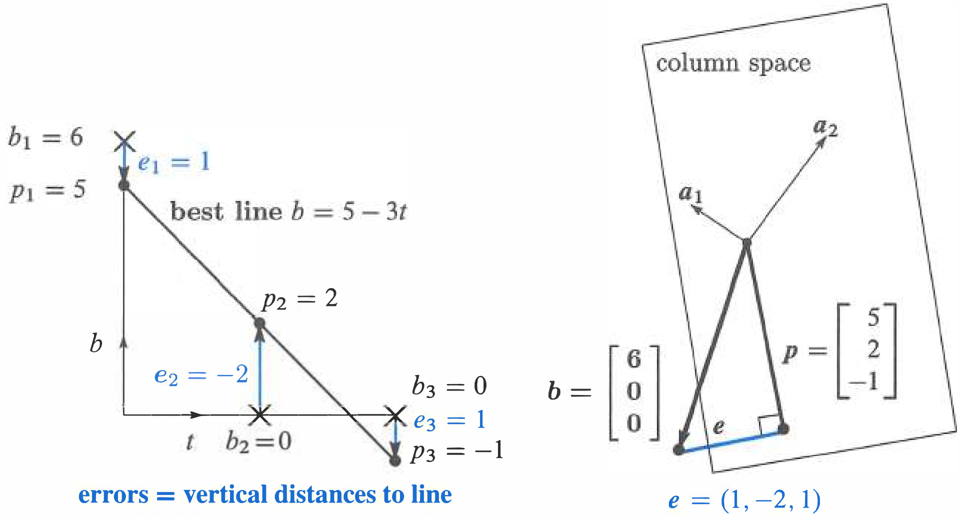


Figure 4.6: **Best line and projection: Two pictures, same problem.** The line has heights $\boldsymbol{p} = (5, 2, -1)$ with errors $\boldsymbol{e} = (1, -2, 1)$. The equations $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$ give $\widehat{\boldsymbol{x}} = (5, -3)$. Same answer! The best line is $b = 5 - 3t$ and the closest point is $\boldsymbol{p} = 5\boldsymbol{a}_1 - 3\boldsymbol{a}_2$.

Notice that the errors $1, -2, 1$ add to zero. *Reason*: The error $\boldsymbol{e} = (e_1, e_2, e_3)$ is perpendicular to the first column $(1, 1, 1)$ in A. The dot product gives $e_1 + e_2 + e_3 = 0$.

By calculus Most functions are minimized by calculus! The graph bottoms out and the derivative in every direction is zero. Here the error function E to be minimized is a *sum of squares* $e_1^2 + e_2^2 + e_3^2$ (the square of the error in each equation):

$$E = \|A\boldsymbol{x} - \boldsymbol{b}\|^2 = (C + D \cdot 0 - 6)^2 + (C + D \cdot 1)^2 + (C + D \cdot 2)^2. \qquad (3)$$

The unknowns are C and D. With two unknowns there are *two derivatives*—both zero at the minimum. They are "partial derivatives" because $\partial E/\partial C$ treats D as constant and $\partial E/\partial D$ treats C as constant:

$$\partial E/\partial C = 2(C + D \cdot 0 - 6) \quad + 2(C + D \cdot 1) \quad + 2(C + D \cdot 2) \quad = 0$$

$$\partial E/\partial D = 2(C + D \cdot 0 - 6)(\mathbf{0}) + 2(C + D \cdot 1)(\mathbf{1}) + 2(C + D \cdot 2)(\mathbf{2}) = 0.$$

$\partial E/\partial D$ contains the extra factors $\mathbf{0}, \mathbf{1}, \mathbf{2}$ from the chain rule. (The last derivative from $(C + 2D)^2$ was 2 times $C + 2D$ times that extra 2.) Those factors are just $\mathbf{1}, \mathbf{1}, \mathbf{1}$ in $\partial E/\partial C$.

It is no accident that those factors 1, 1, 1 and 0, 1, 2 in the derivatives of $||A\boldsymbol{x} - \boldsymbol{b}||^2$ are the columns of A. Now cancel 2 from every term and collect all C's and all D's:

$$\begin{matrix} \text{The } C \text{ derivative is zero:} & 3C + 3D = 6 \\ \text{The } D \text{ derivative is zero:} & 3C + 5D = 0 \end{matrix} \qquad \textbf{This matrix} \begin{bmatrix} 3 & 3 \\ 3 & 5 \end{bmatrix} \textbf{ is } \boldsymbol{A}^{\mathrm{T}}\boldsymbol{A} \tag{4}$$

These equations are identical with $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$. The best C and D are the components of $\widehat{\boldsymbol{x}}$. The equations from calculus are the same as the "normal equations" from linear algebra. These are the key equations of least squares:

The partial derivatives of $||A\boldsymbol{x} - \boldsymbol{b}||^2$ *are zero when* $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\widehat{\boldsymbol{x}} = \boldsymbol{A}^{\mathrm{T}}\boldsymbol{b}$.

The solution is $C = 5$ and $D = -3$. Therefore $b = 5 - 3t$ is the best line—it comes closest to the three points. At $t = 0, 1, 2$ this line goes through $\boldsymbol{p} = 5, 2, -1$. It could not go through $\boldsymbol{b} = 6, 0, 0$. The errors are $1, -2, 1$. This is the vector $\boldsymbol{e}$!

The Big Picture for Least Squares

The key figure of this book shows the four subspaces and the true action of a matrix. The vector $\boldsymbol{x}$ on the left side of Figure 4.3 went to $\boldsymbol{b} = A\boldsymbol{x}$ on the right side. In that figure $\boldsymbol{x}$ was split into $\boldsymbol{x}_r + \boldsymbol{x}_n$. There were *many* solutions to $A\boldsymbol{x} = \boldsymbol{b}$.

In this section the situation is just the opposite. There are *no* solutions to $A\boldsymbol{x} = \boldsymbol{b}$. *Instead of splitting up* $\boldsymbol{x}$ *we are splitting up* $\boldsymbol{b} = \boldsymbol{p} + \boldsymbol{e}$. Figure 4.7 shows the big picture for least squares. Instead of $A\boldsymbol{x} = \boldsymbol{b}$ we solve $A\widehat{\boldsymbol{x}} = \boldsymbol{p}$. The error $\boldsymbol{e} = \boldsymbol{b} - \boldsymbol{p}$ is unavoidable.

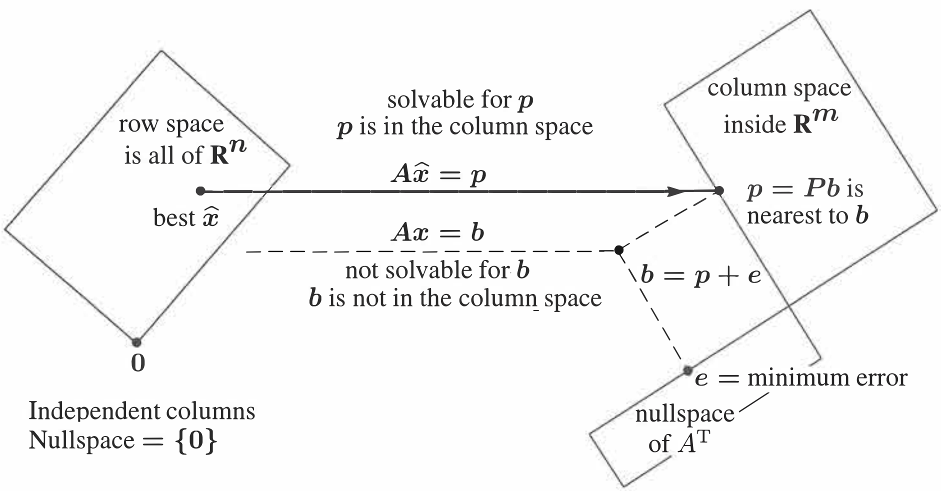


Figure 4.7: The projection $\boldsymbol{p} = A\widehat{\boldsymbol{x}}$ is closest to $\boldsymbol{b}$, so $\widehat{\boldsymbol{x}}$ minimizes $E = ||\boldsymbol{b} - A\boldsymbol{x}||^2$.

Notice how the nullspace $\boldsymbol{N}(A)$ is very small—just one point. With independent columns, the only solution to $A\boldsymbol{x} = \mathbf{0}$ is $\boldsymbol{x} = \mathbf{0}$. Then $A^{\mathrm{T}}A$ is invertible. The equation $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$ fully determines the best vector $\widehat{\boldsymbol{x}}$. The error has $A^{\mathrm{T}}\boldsymbol{e} = \mathbf{0}$.

Chapter 7 will have the complete picture—all four subspaces included. Every $\boldsymbol{x}$ splits into $\boldsymbol{x}_r + \boldsymbol{x}_n$, and every $\boldsymbol{b}$ splits into $\boldsymbol{p} + \boldsymbol{e}$. The best solution is $\widehat{\boldsymbol{x}} = \widehat{\boldsymbol{x}}_r$ in the row space. We can't help $\boldsymbol{e}$ and we don't want $\boldsymbol{x}_n$ from the nullspace—this leaves $A\widehat{\boldsymbol{x}} = \boldsymbol{p}$.

Fitting a Straight Line

Fitting a line is the clearest application of least squares. It starts with $m > 2$ points, hopefully near a straight line. At times $t_1, \ldots, t_m$ those m points are at heights $b_1, \ldots, b_m$. The best line $C + Dt$ misses the points by vertical distances $e_1, \ldots, e_m$. No line is perfect, and the least squares line minimizes $E = e_1^2 + \cdots + e_m^2$.

The first example in this section had three points in Figure 4.6. Now we allow m points (and m can be large). The two components of $\widehat{\boldsymbol{x}}$ are still C and D.

A line goes through the m points when we exactly solve $A\boldsymbol{x} = \boldsymbol{b}$. Generally we can't do it. Two unknowns C and D determine a line, so A has only $n = 2$ columns. To fit the m points, we are trying to solve m equations (and we only have two unknowns!).

$$A\boldsymbol{x} = \boldsymbol{b} \quad \text{is} \quad \begin{aligned} C + Dt_1 &= b_1 \\ C + Dt_2 &= b_2 \\ &\vdots \\ C + Dt_m &= b_m \end{aligned} \qquad \text{with} \qquad A = \begin{bmatrix} 1 & t_1 \\ 1 & t_2 \\ \vdots & \vdots \\ 1 & t_m \end{bmatrix}. \tag{5}$$

The column space is so thin that almost certainly $\boldsymbol{b}$ is outside of it. When $\boldsymbol{b}$ happens to lie in the column space, the points happen to lie on a line. In that case $\boldsymbol{b} = \boldsymbol{p}$. Then $A\boldsymbol{x} = \boldsymbol{b}$ is solvable and the errors are $\boldsymbol{e} = (0, \ldots, 0)$.

The closest line $C + Dt$ has heights $p_1, \ldots, p_m$ with errors $e_1, \ldots, e_m$.

Solve $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$ for $\widehat{\boldsymbol{x}} = (C, D)$. The errors are $e_i = b_i - C - Dt_i$.

Fitting points by a straight line is so important that we give the two equations $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$, once and for all. The two columns of A are independent (unless all times t_i are the same). So we turn to least squares and solve $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$.

$$\textbf{Dot-product matrix} \quad \boldsymbol{A^{\mathrm{T}}A} = \begin{bmatrix} 1 & \cdots & 1 \\ t_1 & \cdots & t_m \end{bmatrix} \begin{bmatrix} 1 & t_1 \\ \vdots & \vdots \\ 1 & t_m \end{bmatrix} = \begin{bmatrix} m & \sum t_i \\ \sum t_i & \sum t_i^2 \end{bmatrix}. \tag{6}$$

On the right side of the normal equation is the 2 by 1 vector $A^{\mathrm{T}}\boldsymbol{b}$:

$$A^{\mathrm{T}}\boldsymbol{b} = \begin{bmatrix} 1 & \cdots & 1 \\ t_1 & \cdots & t_m \end{bmatrix} \begin{bmatrix} b_1 \\ \vdots \\ b_m \end{bmatrix} = \begin{bmatrix} \sum b_i \\ \sum t_i b_i \end{bmatrix}. \tag{7}$$

In a specific problem, these numbers are given. The best $\widehat{\boldsymbol{x}} = (C, D)$ is $(A^{\mathrm{T}}A)^{-1}A^{\mathrm{T}}\boldsymbol{b}$.

The line $C + Dt$ minimizes $e_1^2 + \cdots + e_m^2 = \|A\boldsymbol{x} - \boldsymbol{b}\|^2$ when $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$:

$$A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b} \qquad \begin{bmatrix} m & \sum t_i \\ \sum t_i & \sum t_i^2 \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} \sum b_i \\ \sum t_i b_i \end{bmatrix}. \tag{8}$$

The vertical errors at the m points on the line are the components of $\boldsymbol{e} = \boldsymbol{b} - \boldsymbol{p}$. This error vector (the *residual*) $\boldsymbol{b} - A\widehat{\boldsymbol{x}}$ is perpendicular to the columns of A (geometry). The error is in the nullspace of A^{T} (linear algebra). The best $\widehat{\boldsymbol{x}} = (C, D)$ minimizes the total error E, the sum of squares (calculus):

$$E(\boldsymbol{x}) = \|A\boldsymbol{x} - \boldsymbol{b}\|^2 = (C + Dt_1 - b_1)^2 + \cdots + (C + Dt_m - b_m)^2.$$

Calculus sets the derivatives $\partial E/\partial C$ and $\partial E/\partial D$ to zero, and produces $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$.

Other least squares problems have more than two unknowns. Fitting by the best parabola has $n = 3$ coefficients C, D, E (see below). In general we are fitting m data points by n parameters $x_1, \ldots, x_n$. The matrix A has n columns and $n < m$. The derivatives of $\|A\boldsymbol{x} - \boldsymbol{b}\|^2$ give the n equations $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$. **The derivative of a square is linear.** This is why the method of least squares is so popular.

Example 2 A has *orthogonal columns* when the measurement times t_i add to zero.

Suppose $b = 1, 2, 4$ at times $t = -2, 0, 2$. *Those times add to zero*. The columns of A have *zero dot product*: $(1, 1, 1)$ is orthogonal to $(-2, 0, 2)$:

$$\begin{aligned} C + D(-2) &= 1 \\ C + \quad D(0) &= 2 \\ C + \quad D(2) &= 4 \end{aligned} \qquad \text{or} \qquad A\boldsymbol{x} = \begin{bmatrix} 1 & -2 \\ 1 & 0 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 4 \end{bmatrix}.$$

When the columns of A are orthogonal, $A^{\mathrm{T}}A$ will be a diagonal matrix:

$$A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b} \qquad \text{is} \qquad \begin{bmatrix} 3 & \mathbf{0} \\ \mathbf{0} & 8 \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} 7 \\ 6 \end{bmatrix}. \tag{9}$$

Main point: Since $A^{\mathrm{T}}A$ *is diagonal*, we can solve separately for $C = \frac{7}{3}$ and $D = \frac{6}{8}$. The zeros in $A^{\mathrm{T}}A$ are dot products of perpendicular columns in A. The diagonal matrix $A^{\mathrm{T}}A$, with entries $m = 3$ and $t_1^2 + t_2^2 + t_3^2 = 8$, is virtually as good as the identity matrix.

Orthogonal columns are so helpful that it is worth *shifting the times by subtracting the average time* $\widehat{t} = (t_1 + \cdots + t_m)/m$. If the original times were $1, 3, 5$ then their average is $\widehat{t} = 3$. The shifted times $T = t - \widehat{t} = t - 3$ add up to zero!

$$\begin{aligned} T_1 &= 1 - 3 = -2 \\ T_2 &= 3 - 3 = \ \ 0 \\ T_3 &= 5 - 3 = \ \ 2 \end{aligned} \qquad A_{\text{new}} = \begin{bmatrix} 1 & T_1 \\ 1 & T_2 \\ 1 & T_3 \end{bmatrix} \qquad A_{\text{new}}^{\mathrm{T}}A_{\text{new}} = \begin{bmatrix} 3 & \mathbf{0} \\ \mathbf{0} & 8 \end{bmatrix}.$$

Now C and D come from the easy equation (9). Then the best straight line uses $C + DT$ which is $C + D(t - \widehat{t}\,) = C + D(t - 3)$. Problem 30 even gives a formula for C and D.

That was a perfect example of the "Gram-Schmidt idea" coming in the next section: *Make the columns orthogonal in advance*. Then $A_{\text{new}}^{\mathrm{T}} A_{\text{new}}$ is diagonal and $\widehat{\boldsymbol{x}}_{\text{new}}$ is easy.

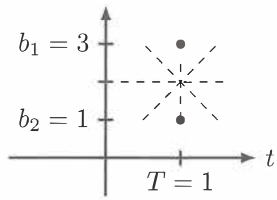
Dependent Columns in A: What is $\widehat{\boldsymbol{x}}$?

From the start, this chapter has assumed independent columns in A. Then $A^{\mathrm{T}}A$ is invertible. Then $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$ produces the least squares solution to $A\boldsymbol{x} = \boldsymbol{b}$.

Which $\widehat{\boldsymbol{x}}$ is best if A has *dependent columns*? Here is a specific example.

$$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 3 \\ 1 \end{bmatrix} = \boldsymbol{b} \qquad\qquad \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} \widehat{x}_1 \\ \widehat{x}_2 \end{bmatrix} = \begin{bmatrix} 2 \\ 2 \end{bmatrix} = \boldsymbol{p}$$

$$A\boldsymbol{x} = \boldsymbol{b} \qquad\qquad\qquad A\widehat{\boldsymbol{x}} = \boldsymbol{p}$$



The measurements $b_1 = 3$ and $b_2 = 1$ are at the same time T! A straight line $C + Dt$ cannot go through both points. I think we are right to project $\boldsymbol{b} = (3, 1)$ to $\boldsymbol{p} = (2, 2)$ in the column space of A. That changes the equation $A\boldsymbol{x} = \boldsymbol{b}$ to the equation $A\widehat{\boldsymbol{x}} = \boldsymbol{p}$. An equation with no solution has become an equation with infinitely many solutions. The problem is that A has dependent columns and $(1, -1)$ is in its nullspace.

Which solution $\widehat{\boldsymbol{x}}$ should we choose? All the dashed lines in the figure have the same two errors 1 and -1 at time T. Those errors $(1, -1) = \boldsymbol{e} = \boldsymbol{b} - \boldsymbol{p}$ are as small as possible. But this doesn't tell us which dashed line is best.

My instinct is to go for the horizontal line at height 2. If the equation for the best line is $b = C + Dt$, then my choice will have $\widehat{x}_1 = C = 2$ and $\widehat{x}_2 = D = 0$. But what if the line had been written as $b = ct + d$? This is equally correct (just reversing C and D). Now the horizontal line has $\widehat{x}_1 = c = 0$ and $\widehat{x}_2 = d = 2$. I don't see any way out.

In Section 7.4, the *"pseudoinverse" of A* will choose the **shortest solution to** $A\widehat{\boldsymbol{x}} = \boldsymbol{p}$. Here, that shortest solution will be $\boldsymbol{x}^+ = (1, 1)$. This is the particular solution in the row space of A, and $\boldsymbol{x}^+$ has length $\sqrt{2}$. (Both solutions $\widehat{\boldsymbol{x}} = (2, 0)$ and $(0, 2)$ have length 2.) We are arbitrarily choosing the nullspace component of the solution $\boldsymbol{x}^+$ to be zero.

When A has independent columns, the nullspace only contains the zero vector and the pseudoinverse is our usual left inverse $L = (A^{\mathrm{T}}A)^{-1}A^{\mathrm{T}}$. When I write it that way, the pseudoinverse sounds like the best way to choose $\boldsymbol{x}$.

Comment MATLAB experiments with singular matrices produced either **Inf** or **NaN** (Not a Number) or $\mathbf{10^{16}}$ (a bad number). There is a warning in every case! I believe that **Inf** and **NaN** and $\mathbf{10^{16}}$ come from the possibilities $\mathbf{0}\boldsymbol{x} = \boldsymbol{b}$ and $\mathbf{0}\boldsymbol{x} = \mathbf{0}$ and $\mathbf{10^{-16}}\,\boldsymbol{x} = \mathbf{1}$.

Those are three small examples of three big difficulties: singular with no solution, singular with many solutions, and very very close to singular.

Fitting by a Parabola

If we throw a ball, it would be crazy to fit the path by a straight line. A parabola $b = C + Dt + Et^2$ allows the ball to go up and come down again (b is the height at time t). The actual path is not a perfect parabola, but the whole theory of projectiles starts with that approximation.

When Galileo dropped a stone from the Leaning Tower of Pisa, it accelerated. The distance contains a quadratic term $\frac{1}{2}gt^2$. (Galileo's point was that the stone's mass is not involved.) Without that t^2 term we could never send a satellite into its orbit. But even with a nonlinear function like t^2, the unknowns C, D, E still appear linearly! Fitting points by the best parabola is still a problem in linear algebra.

Problem Fit heights $b_1, \ldots, b_m$ at times $t_1, \ldots, t_m$ by a parabola $C + Dt + Et^2$.

Solution With $m > 3$ points, the m equations for an exact fit are generally unsolvable:

$$\begin{aligned} C + Dt_1 + Et_1^2 &= b_1 \\ &\vdots \\ C + Dt_m + Et_m^2 &= b_m \end{aligned} \qquad \text{is } A\boldsymbol{x} = \boldsymbol{b} \text{ with the } m \text{ by 3 matrix} \qquad A = \begin{bmatrix} 1 & t_1 & t_1^2 \\ \vdots & \vdots & \vdots \\ 1 & t_m & t_m^2 \end{bmatrix}. \tag{10}$$

Least squares The closest parabola $C + Dt + Et^2$ chooses $\widehat{\boldsymbol{x}} = (C, D, E)$ to satisfy the three normal equations $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$.

May I ask you to convert this to a problem of projection? The column space of A has dimension _____. The projection of $\boldsymbol{b}$ is $\boldsymbol{p} = A\widehat{\boldsymbol{x}}$, which combines the three columns using the coefficients C, D, E. The error at the first data point is $e_1 = b_1 - C - Dt_1 - Et_1^2$. The total squared error is $e_1^2 +$ _____. If you prefer to minimize by calculus, take the partial derivatives of E with respect to _____, _____, _____. These three derivatives will be zero when $\widehat{\boldsymbol{x}} = (C, D, E)$ solves the 3 by 3 system of equations $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$.

Section 10.5 has more least squares applications. The big one is Fourier series—approximating functions instead of vectors. The function to be minimized changes from a sum of squared errors $e_1^2 + \cdots + e_m^2$ to an integral of the squared error.

Example 3 For a parabola $b = C + Dt + Et^2$ to go through the three heights $b = 6, 0, 0$ when $t = 0, 1, 2$, the equations for C, D, E are

$$\begin{aligned} C + D \cdot 0 + E \cdot 0^2 &= 6 \\ C + D \cdot 1 + E \cdot 1^2 &= 0 \\ C + D \cdot 2 + E \cdot 2^2 &= 0. \end{aligned} \tag{11}$$

This is $A\boldsymbol{x} = \boldsymbol{b}$. We can solve it exactly. Three data points give three equations and a square matrix. The solution is $\boldsymbol{x} = (C, D, E) = (\mathbf{6}, \mathbf{-9}, \mathbf{3})$. The parabola through the three points in Figure 4.8a is $b = \mathbf{6 - 9}\boldsymbol{t} + \mathbf{3}\boldsymbol{t}^{\mathbf{2}}$.

What does this mean for projection? The matrix has three columns, which span the whole space $\mathbf{R}^3$. The projection matrix is the identity. The projection of $\boldsymbol{b}$ is $\boldsymbol{b}$. The error is zero. We didn't need $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$, because we solved $A\boldsymbol{x} = \boldsymbol{b}$. Of course we could multiply by A^{T}, but there is no reason to do it.

Figure 4.8 also shows a fourth point b_4 at time t_4. If that falls on the parabola, the new $A\boldsymbol{x} = \boldsymbol{b}$ (four equations) is still solvable. When the fourth point is not on the parabola, we turn to $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$. Will the least squares parabola stay the same, with all the error at the fourth point? Not likely!

Least squares balances the four errors to get three equations for C, D, E.

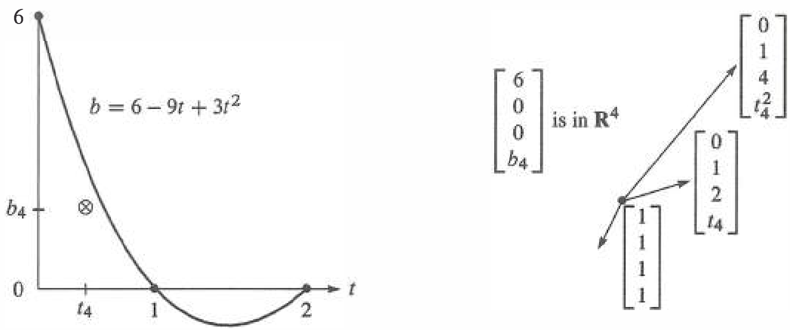


Figure 4.8: An exact fit of the parabola at $t = 0, 1, 2$ means that $\boldsymbol{p} = \boldsymbol{b}$ and $\boldsymbol{e} = \mathbf{0}$. The fourth point ⓧ off the parabola makes $m > n$ and we need least squares: project $\boldsymbol{b}$ on $\boldsymbol{C}(\boldsymbol{A})$. The figure on the right shows $\boldsymbol{b}$—not a combination of the three columns of A.

■ REVIEW OF THE KEY IDEAS ■

1. The least squares solution $\widehat{\boldsymbol{x}}$ minimizes $\|A\boldsymbol{x} - \boldsymbol{b}\|^2 = \boldsymbol{x}^{\mathrm{T}}A^{\mathrm{T}}A\boldsymbol{x} - 2\boldsymbol{x}^{\mathrm{T}}A^{\mathrm{T}}\boldsymbol{b} + \boldsymbol{b}^{\mathrm{T}}\boldsymbol{b}$. This is E, the sum of squares of the errors in the m equations $(m > n)$.

2. The best $\widehat{\boldsymbol{x}}$ comes from the normal equations $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$. E is a minimum.

3. To fit m points by a line $b = C + Dt$, the normal equations give C and D.

4. The heights of the best line are $\boldsymbol{p} = (p_1, \ldots, p_m)$. The vertical distances to the data points are the errors $\boldsymbol{e} = (e_1, \ldots, e_m)$. A key equation is $A^{\mathrm{T}}\boldsymbol{e} = \mathbf{0}$.

5. If we try to fit m points by a combination of $n < m$ functions, the m equations $A\boldsymbol{x} = \boldsymbol{b}$ are generally unsolvable. The n equations $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$ give the least squares solution—the combination with smallest MSE (mean square error).

■ WORKED EXAMPLES ■

4.3 A Start with nine measurements b_1 to b_9, *all zero*, at times $t = 1, \ldots, 9$. The tenth measurement $b_{10} = 40$ is an outlier. Find the **best horizontal line** $\boldsymbol{y = C}$ to fit the ten points $(1, 0), (2, 0), \ldots, (9, 0), (10, 40)$ using three options for the error E:

(1) Least *squares* $E_2 = e_1^2 + \cdots + e_{10}^2$ (then the normal equation for C is linear)

(2) Least *maximum* error $E_\infty = |e_{\max}|$ **(3)** Least *sum* of errors $E_1 = |e_1| + \cdots + |e_{10}|$.

Solution (1) The least squares fit to $0, 0, \ldots, 0, 40$ by a horizontal line is $\boldsymbol{C = 4}$:

$$A = \text{column of 1's} \quad A^{\mathrm{T}}A = 10 \quad A^{\mathrm{T}}\boldsymbol{b} = \text{sum of } b_i = 40. \quad \text{So } 10\,C = 40.$$

(2) The least maximum error requires $\boldsymbol{C = 20}$, halfway between 0 and 40.

(3) The least sum requires $\boldsymbol{C = 0}$ (!!). The sum of errors $9|C| + |40 - C|$ would increase if C moves up from zero.

The least sum comes from the *median* measurement (the median of $0, \ldots, 0, 40$ is zero). Many statisticians feel that the least squares solution is too heavily influenced by outliers like $b_{10} = 40$, and they prefer least sum. But the equations become *nonlinear*.

Now find the least squares line $C + Dt$ through those ten points $(1, 0)$ to $(10, 40)$:

$$A^{\mathrm{T}}A = \begin{bmatrix} 10 & \sum t_i \\ \sum t_i & \sum t_i^2 \end{bmatrix} = \begin{bmatrix} 10 & 55 \\ 55 & 385 \end{bmatrix} \qquad A^{\mathrm{T}}\boldsymbol{b} = \begin{bmatrix} \sum b_i \\ \sum t_i b_i \end{bmatrix} = \begin{bmatrix} 40 \\ 400 \end{bmatrix}$$

Those come from equation (8). Then $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$ gives $C = -8$ and $D = 24/11$.

What happens to C and D if you multiply $\boldsymbol{b} = (0, 0, \ldots, 40)$ by 3 and then add 30 to get $\boldsymbol{b}_{\text{new}} = (30, 30, \ldots, 150)$? Linearity allows us to rescale $\boldsymbol{b}$. Multiplying $\boldsymbol{b}$ by 3 will multiply C and D by 3. Adding 30 to all b_i will add 30 to C.

4.3 B Find the parabola $C + Dt + Et^2$ that comes closest (least squares error) to the values $\boldsymbol{b} = (0, 0, 1, 0, 0)$ at the times $t = -2, -1, 0, 1, 2$. First write down the five equations $A\boldsymbol{x} = \boldsymbol{b}$ in three unknowns $\boldsymbol{x} = (C, D, E)$ for a parabola to go through the five points. No solution because no such parabola exists. Solve $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$.

I would predict $D = 0$. Why should the best parabola be symmetric around $t = 0$? In $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$, equation 2 for D should uncouple from equations 1 and 3.

Solution The five equations $A\boldsymbol{x} = \boldsymbol{b}$ have a rectangular *Vandermonde matrix* A:

$$\begin{aligned} C + D\,(-2) + E\,(-2)^2 &= 0 \\ C + D\,(-1) + E\,(-1)^2 &= 0 \\ C + D\,\ (0) + E\,\ (0)^2 &= 1 \\ C + D\,\ (1) + E\,\ (1)^2 &= 0 \\ C + D\,\ (2) + E\,\ (2)^2 &= 0 \end{aligned} \qquad A = \begin{bmatrix} 1 & -2 & 4 \\ 1 & -1 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 2 & 4 \end{bmatrix} \qquad A^{\mathrm{T}}A = \begin{bmatrix} 5 & \mathbf{0} & 10 \\ \mathbf{0} & 10 & \mathbf{0} \\ 10 & \mathbf{0} & 34 \end{bmatrix}$$

Those zeros in $A^{\mathrm{T}}A$ mean that column 2 of A is orthogonal to columns 1 and 3. We see this directly in A (the times $-2, -1, 0, 1, 2$ are symmetric). The best C, D, E in the parabola $C + Dt + Et^2$ come from $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$, and D is uncoupled from C and E:

$$\begin{bmatrix} 5 & 0 & 10 \\ 0 & 10 & 0 \\ 10 & 0 & 34 \end{bmatrix} \begin{bmatrix} C \\ D \\ E \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad \text{leads to} \quad \begin{array}{l} C = 34/70 \\ D = 0 \ \text{ as predicted} \\ E = -10/70 \end{array}$$

Problem Set 4.3

Problems 1–11 use four data points $\boldsymbol{b} = (0, 8, 8, 20)$ to bring out the key ideas.

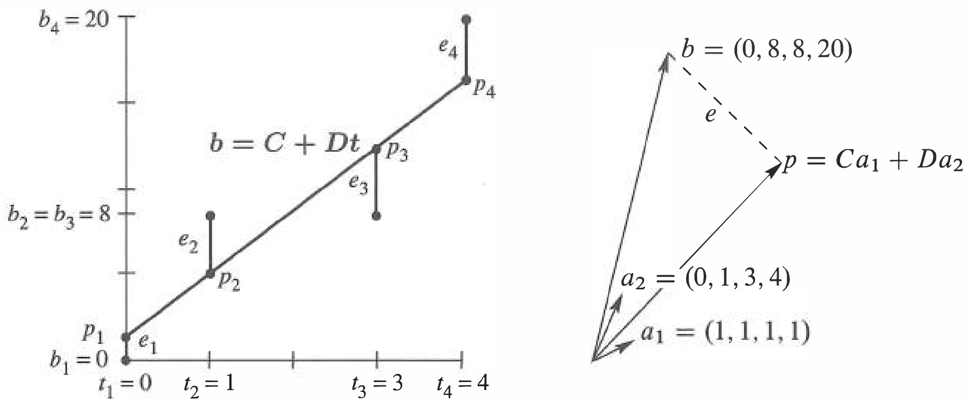


Figure 4.9: **Problems 1–11**: The closest line $C + Dt$ matches $C\boldsymbol{a}_1 + D\boldsymbol{a}_2$ in $\mathbf{R}^4$.

1 With $b = 0, 8, 8, 20$ at $t = 0, 1, 3, 4$, set up and solve the normal equations $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$. For the best straight line in Figure 4.9a, find its four heights p_i and four errors e_i. What is the minimum value $E = e_1^2 + e_2^2 + e_3^2 + e_4^2$?

2 (Line $C + Dt$ does go through p's) With $b = 0, 8, 8, 20$ at times $t = 0, 1, 3, 4$, write down the four equations $A\boldsymbol{x} = \boldsymbol{b}$ (unsolvable). Change the measurements to $p = 1, 5, 13, 17$ and find an exact solution to $A\widehat{\boldsymbol{x}} = \boldsymbol{p}$.

3 Check that $\boldsymbol{e} = \boldsymbol{b} - \boldsymbol{p} = (-1, 3, -5, 3)$ is perpendicular to both columns of the same matrix A. What is the shortest distance $\|\boldsymbol{e}\|$ from $\boldsymbol{b}$ to the column space of A?

4 (By calculus) Write down $E = \|A\boldsymbol{x} - \boldsymbol{b}\|^2$ as a sum of four squares—the last one is $(C + 4D - 20)^2$. Find the derivative equations $\partial E/\partial C = 0$ and $\partial E/\partial D = 0$. Divide by 2 to obtain the normal equations $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$.

5 Find the height C of the best *horizontal line* to fit $\boldsymbol{b} = (0, 8, 8, 20)$. An exact fit would solve the unsolvable equations $C = 0$, $C = 8$, $C = 8$, $C = 20$. Find the 4 by 1 matrix A in these equations and solve $A^{\mathrm{T}}A\widehat{x} = A^{\mathrm{T}}\boldsymbol{b}$. Draw the horizontal line at height $\widehat{x} = C$ and the four errors in $\boldsymbol{e}$.

6 Project $\boldsymbol{b} = (0, 8, 8, 20)$ onto the line through $\boldsymbol{a} = (1, 1, 1, 1)$. Find $\widehat{x} = \boldsymbol{a}^{\mathrm{T}}\boldsymbol{b}/\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a}$ and the projection $\boldsymbol{p} = \widehat{x}\boldsymbol{a}$. Check that $\boldsymbol{e} = \boldsymbol{b} - \boldsymbol{p}$ is perpendicular to $\boldsymbol{a}$, and find the shortest distance $\|\boldsymbol{e}\|$ from $\boldsymbol{b}$ to the line through $\boldsymbol{a}$.

7 Find the closest line $b = Dt$, *through the origin*, to the same four points. An exact fit would solve $D \cdot 0 = 0, D \cdot 1 = 8, D \cdot 3 = 8, D \cdot 4 = 20$. Find the 4 by 1 matrix and solve $A^{\mathrm{T}}A\widehat{x} = A^{\mathrm{T}}\boldsymbol{b}$. Redraw Figure 4.9a showing the best line $b = Dt$ and the e's.

8 Project $\boldsymbol{b} = (0, 8, 8, 20)$ onto the line through $\boldsymbol{a} = (0, 1, 3, 4)$. Find $\widehat{x} = D$ and $\boldsymbol{p} = \widehat{x}\boldsymbol{a}$. The best C in Problems 5–6 and the best D in Problems 7–8 do *not* agree with the best (C, D) in Problems 1–4. That is because $(1, 1, 1, 1)$ and $(0, 1, 3, 4)$ are ______ perpendicular.

9 For the closest parabola $b = C + Dt + Et^2$ to the same four points, write down the unsolvable equations $A\boldsymbol{x} = \boldsymbol{b}$ in three unknowns $\boldsymbol{x} = (C, D, E)$. Set up the three normal equations $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$ (solution not required). In Figure 4.9a you are now fitting a parabola to 4 points—what is happening in Figure 4.9b?

10 For the closest cubic $b = C + Dt + Et^2 + Ft^3$ to the same four points, write down the four equations $A\boldsymbol{x} = \boldsymbol{b}$. Solve them by elimination. In Figure 4.9a this cubic now goes exactly through the points. What are $\boldsymbol{p}$ and $\boldsymbol{e}$?

11 The average of the four times is $\widehat{t} = \frac{1}{4}(0 + 1 + 3 + 4) = 2$. The average of the four b's is $\widehat{b} = \frac{1}{4}(0 + 8 + 8 + 20) = 9$.

(a) Verify that the best line goes through the center point $(\widehat{t}, \widehat{b}) = (2, 9)$.

(b) Explain why $C + D\widehat{t} = \widehat{b}$ comes from the first equation in $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$.

Questions 12–16 introduce basic ideas of statistics—the foundation for least squares.

12 (Recommended) This problem projects $\boldsymbol{b} = (b_1, \ldots, b_m)$ onto the line through $\boldsymbol{a} = (1, \ldots, 1)$. We solve m equations $\boldsymbol{a}x = \boldsymbol{b}$ in 1 unknown (by least squares).

(a) Solve $\boldsymbol{a}^{\mathrm{T}}\boldsymbol{a}\widehat{x} = \boldsymbol{a}^{\mathrm{T}}\boldsymbol{b}$ to show that $\widehat{x}$ is the *mean* (the average) of the $\boldsymbol{b}$'s.

(b) Find $\boldsymbol{e} = \boldsymbol{b} - \boldsymbol{a}\widehat{x}$ and the *variance* $\|\boldsymbol{e}\|^2$ and the *standard deviation* $\|\boldsymbol{e}\|$.

(c) The horizontal line $\widehat{\boldsymbol{b}} = 3$ is closest to $\boldsymbol{b} = (1, 2, 6)$. Check that $\boldsymbol{p} = (3, 3, 3)$ is perpendicular to $\boldsymbol{e}$ and find the 3 by 3 projection matrix P.

13 First assumption behind least squares: $A\boldsymbol{x} = \boldsymbol{b}-$ ***(noise e with mean zero)***. Multiply the error vectors $\boldsymbol{e} = \boldsymbol{b} - A\boldsymbol{x}$ by $(A^{\mathrm{T}}A)^{-1}A^{\mathrm{T}}$ to get $\widehat{\boldsymbol{x}} - \boldsymbol{x}$ on the right. The estimation errors $\widehat{\boldsymbol{x}} - \boldsymbol{x}$ also average to zero. The estimate $\widehat{\boldsymbol{x}}$ is *unbiased.*

14 Second assumption behind least squares: The m errors $\boldsymbol{e}_i$ are independent with variance σ^2, so the average of $(\boldsymbol{b} - A\boldsymbol{x})(\boldsymbol{b} - A\boldsymbol{x})^{\mathrm{T}}$ is $\sigma^2 I$. Multiply on the left by $(A^{\mathrm{T}}A)^{-1}A^{\mathrm{T}}$ and on the right by $A(A^{\mathrm{T}}A)^{-1}$ to show that the average matrix $(\widehat{\boldsymbol{x}} - \boldsymbol{x})(\widehat{\boldsymbol{x}} - \boldsymbol{x})^{\mathrm{T}}$ is $\sigma^2(A^{\mathrm{T}}A)^{-1}$. This is the ***covariance matrix*** W in Section 10.2.

15 A doctor takes 4 readings of your heart rate. The best solution to $x = b_1, \ldots, x = b_4$ is the average $\widehat{x}$ of $b_1, \ldots, b_4$. The matrix A is a column of 1's. Problem 14 gives the expected error $(\widehat{x} - x)^2$ as $\sigma^2(A^{\mathrm{T}}A)^{-1} =$ ____. ***By averaging, the variance drops from σ^2 to $\sigma^2/4$.***

16 If you know the average $\widehat{x}_9$ of 9 numbers $b_1, \ldots, b_9$, how can you quickly find the average $\widehat{x}_{10}$ with one more number b_{10}? The idea of *recursive* least squares is to avoid adding 10 numbers. What number multiplies $\widehat{x}_9$ in computing $\widehat{x}_{10}$?

$$\widehat{x}_{10} = \tfrac{1}{10}b_{10} + \underline{\qquad}\,\widehat{x}_9 = \tfrac{1}{10}(b_1 + \cdots + b_{10}) \quad \text{as in Worked Example 4.2 C.}$$

Questions 17–24 give more practice with $\widehat{\boldsymbol{x}}$ and $\boldsymbol{p}$ and $\boldsymbol{e}$.

17 Write down three equations for the line $b = C + Dt$ to go through $b = 7$ at $t = -1$, $b = 7$ at $t = 1$, and $b = 21$ at $t = 2$. Find the least squares solution $\widehat{\boldsymbol{x}} = (C, D)$ and draw the closest line.

18 Find the projection $\boldsymbol{p} = A\widehat{\boldsymbol{x}}$ in Problem 17. This gives the three heights of the closest line. Show that the error vector is $\boldsymbol{e} = (2, -6, 4)$. Why is $P\boldsymbol{e} = \boldsymbol{0}$?

19 Suppose the measurements at $t = -1, 1, 2$ are the errors $2, -6, 4$ in Problem 18. Compute $\widehat{\boldsymbol{x}}$ and the closest line to these new measurements. Explain the answer: $\boldsymbol{b} = (2, -6, 4)$ is perpendicular to ____ so the projection is $\boldsymbol{p} = \boldsymbol{0}$.

20 Suppose the measurements at $t = -1, 1, 2$ are $\boldsymbol{b} = (5, 13, 17)$. Compute $\widehat{\boldsymbol{x}}$ and the closest line and $\boldsymbol{e}$. The error is $\boldsymbol{e} = \boldsymbol{0}$ because this $\boldsymbol{b}$ is ____.

21 Which of the four subspaces contains the error vector $\boldsymbol{e}$? Which contains $\boldsymbol{p}$? Which contains $\widehat{\boldsymbol{x}}$? What is the nullspace of A?

22 Find the best line $C + Dt$ to fit $b = 4, 2, -1, 0, 0$ at times $t = -2, -1, 0, 1, 2$.

23 Is the error vector $\boldsymbol{e}$ orthogonal to $\boldsymbol{b}$ or $\boldsymbol{p}$ or $\boldsymbol{e}$ or $\widehat{\boldsymbol{x}}$? Show that $\|\boldsymbol{e}\|^2$ equals $\boldsymbol{e}^{\mathrm{T}}\boldsymbol{b}$ which equals $\boldsymbol{b}^{\mathrm{T}}\boldsymbol{b} - \boldsymbol{p}^{\mathrm{T}}\boldsymbol{b}$. This is the smallest total error E.

24 The partial derivatives of $\|A\boldsymbol{x}\|^2$ with respect to $x_1, \ldots, x_n$ fill the vector $2A^{\mathrm{T}}A\boldsymbol{x}$. The derivatives of $2\boldsymbol{b}^{\mathrm{T}}A\boldsymbol{x}$ fill the vector $2A^{\mathrm{T}}\boldsymbol{b}$. So the derivatives of $\|A\boldsymbol{x} - \boldsymbol{b}\|^2$ are zero when ____.

Challenge Problems

25 *What condition on $(t_1, b_1), (t_2, b_2), (t_3, b_3)$ puts those three points onto a straight line*? A column space answer is: (b_1, b_2, b_3) must be a combination of $(1, 1, 1)$ and (t_1, t_2, t_3). Try to reach a specific equation connecting the t's and b's. I should have thought of this question sooner!

26 Find the *plane* that gives the best fit to the 4 values $\boldsymbol{b} = (0, 1, 3, 4)$ at the corners $(1, 0)$ and $(0, 1)$ and $(-1, 0)$ and $(0, -1)$ of a square. The equations $C + Dx + Ey = b$ at those 4 points are $A\boldsymbol{x} = \boldsymbol{b}$ with 3 unknowns $\boldsymbol{x} = (C, D, E)$. What is A? At the center $(0, 0)$ of the square, show that $C + Dx + Ey =$ average of the b's.

27 (Distance between lines) The points $P = (x, x, x)$ and $Q = (y, 3y, -1)$ are on two lines in space that don't meet. Choose x and y to minimize the squared distance $\|P - Q\|^2$. The line connecting the closest P and Q is perpendicular to _____.

28 Suppose the columns of A are not independent. How could you find a matrix B so that $P = B(B^{\mathrm{T}}B)^{-1}B^{\mathrm{T}}$ does give the projection onto the column space of A? (The usual formula will fail when $A^{\mathrm{T}}A$ is not invertible.)

29 Usually there will be exactly one hyperplane in $\mathbf{R}^n$ that contains the n given points $\boldsymbol{x} = \mathbf{0}, \boldsymbol{a}_1, \ldots, \boldsymbol{a}_{n-1}$. (Example for $n = 3$: There will be one plane containing $0, \boldsymbol{a}_1, \boldsymbol{a}_2$ unless _____.) What is the test to have exactly one plane in $\mathbf{R}^n$?

30 Example 2 shifted the times t_i to make them add to zero. We subtracted away the average time $\widehat{t} = (t_1 + \cdots + t_m)/m$ to get $T_i = t_i - \widehat{t}$. Those T_i add to zero.

With the columns $(1, \ldots, 1)$ and $(T_1, \ldots, T_m)$ now orthogonal, $A^{\mathrm{T}}A$ is diagonal. Its entries are m and $T_1^2 + \cdots + T_m^2$. Show that the best C and D have direct formulas:

$$\boldsymbol{T} \textbf{ is } \boldsymbol{t} - \widehat{\boldsymbol{t}} \qquad C = \frac{b_1 + \cdots + b_m}{m} \qquad \text{and} \qquad D = \frac{b_1T_1 + \cdots + b_mT_m}{T_1^2 + \cdots + T_m^2}.$$

The best line is $C + DT$ ***or*** $C + D(t - \widehat{t})$. The time shift that makes $A^{\mathrm{T}}A$ diagonal is an example of the Gram-Schmidt process: *orthogonalize the columns of A in advance*.

4.4 Orthonormal Bases and Gram-Schmidt

1 The columns $q_1, \ldots, q_n$ are orthonormal if $\boldsymbol{q}_i^{\mathrm{T}}\boldsymbol{q}_j = \left\{ \begin{array}{l} 0 \text{ for } i \neq j \\ 1 \text{ for } i = j \end{array} \right\}$. Then $\boxed{Q^{\mathrm{T}}Q = I\,.}$

2 If Q is also square, then $QQ^{\mathrm{T}} = I$ and $\boxed{Q^{\mathrm{T}} = Q^{-1}}$. Q is an "orthogonal matrix".

3 The least squares solution to $Q\boldsymbol{x} = \boldsymbol{b}$ is $\widehat{\boldsymbol{x}} = Q^{\mathrm{T}}\boldsymbol{b}$. Projection of $\boldsymbol{b}$: $\boldsymbol{p} = QQ^{\mathrm{T}}\boldsymbol{b} = P\boldsymbol{b}$.

4 The **Gram-Schmidt** process takes independent $\boldsymbol{a}_i$ to orthonormal $\boldsymbol{q}_i$. Start with $\boldsymbol{q}_1 = \boldsymbol{a}_1 / \,||\boldsymbol{a}_1||$.

5 $\boldsymbol{q}_i$ is $(\boldsymbol{a}_i -$ projection $\boldsymbol{p}_i) \,/\, ||\boldsymbol{a}_i - \boldsymbol{p}_i||$; projection $\boldsymbol{p}_i = (\boldsymbol{a}_i^{\mathrm{T}}\boldsymbol{q}_1)\boldsymbol{q}_1 + \cdots + (\boldsymbol{a}_i^{\mathrm{T}}\boldsymbol{q}_{i-1})\boldsymbol{q}_{i-1}$.

6 Each $\boldsymbol{a}_i$ will be a combination of $\boldsymbol{q}_1$ to $\boldsymbol{q}_i$. Then $\boldsymbol{A} = \boldsymbol{QR}$: orthogonal Q and triangular R.

This section has two goals, **why** and **how**. The first is to see why orthogonality is good. Dot products are zero, so $A^{\mathrm{T}}A$ will be diagonal. It becomes so easy to find $\widehat{\boldsymbol{x}}$ and $\boldsymbol{p} = A\widehat{\boldsymbol{x}}$. ***The second goal is to construct orthogonal vectors.*** You will see how Gram-Schmidt chooses combinations of the original basis vectors to produce right angles. Those original vectors are the columns of A, probably *not* orthogonal. ***The orthonormal basis vectors will be the columns of a new matrix Q.***

From Chapter 3, a basis consists of independent vectors that span the space. The basis vectors could meet at any angle (except $0°$ and $180°$). But every time we visualize axes, they are perpendicular. *In our imagination, the coordinate axes are practically always orthogonal.* This simplifies the picture and it greatly simplifies the computations.

The vectors $\boldsymbol{q}_1, \ldots, \boldsymbol{q}_n$ are ***orthogonal*** when their dot products $\boldsymbol{q}_i \cdot \boldsymbol{q}_j$ are zero. More exactly $\boldsymbol{q}_i^{\mathrm{T}}\boldsymbol{q}_j = 0$ whenever $i \neq j$. With one more step—just *divide each vector by its length*—the vectors become ***orthogonal unit vectors***. Their lengths are all 1 (normal). Then the basis is called ***orthonormal***.

DEFINITION The vectors $\boldsymbol{q}_1, \ldots, \boldsymbol{q}_n$ are ***orthonormal*** if

$$\boldsymbol{q}_i^{\mathrm{T}}\boldsymbol{q}_j = \begin{cases} 0 & \text{when } i \neq j \quad (\textbf{\textit{orthogonal}} \text{ vectors}) \\ 1 & \text{when } i = j \quad (\textbf{\textit{unit}} \text{ vectors: } ||\boldsymbol{q}_i|| = 1) \end{cases}$$

A matrix with orthonormal columns is assigned the special letter Q.

The matrix Q is easy to work with because $Q^{\mathrm{T}}Q = I$. This repeats in matrix language that the columns $\boldsymbol{q}_1, \ldots, \boldsymbol{q}_n$ are orthonormal. Q is not required to be square.

A matrix Q with orthonormal columns satisfies $\boxed{Q^{\mathrm{T}}Q = I}$ **:**

$$\boxed{Q^{\mathrm{T}}Q} = \begin{bmatrix} - \boldsymbol{q}_1^{\mathrm{T}} - \\ - \boldsymbol{q}_2^{\mathrm{T}} - \\ \\ - \boldsymbol{q}_n^{\mathrm{T}} - \end{bmatrix} \begin{bmatrix} | & | & & | \\ \boldsymbol{q}_1 & \boldsymbol{q}_2 & & \boldsymbol{q}_n \\ | & | & & | \end{bmatrix} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix} = \boxed{I}\,. \quad (1)$$

When row i of Q^{T} multiplies column j of Q, the dot product is $\boldsymbol{q}_i^{\mathrm{T}}\boldsymbol{q}_j$. Off the diagonal $(i \neq j)$ that dot product is zero by orthogonality. On the diagonal $(i = j)$ the unit vectors give $\boldsymbol{q}_i^{\mathrm{T}}\boldsymbol{q}_i = \|\boldsymbol{q}_i\|^2 = 1$. Often Q is rectangular $(m > n)$. Sometimes $m = n$.

When Q is square, $Q^{\mathrm{T}}Q = I$ means that $Q^{\mathrm{T}} = Q^{-1}$: transpose = inverse.

If the columns are only orthogonal (not unit vectors), dot products still give a diagonal matrix (not the identity matrix). This diagonal matrix is almost as good as I. The important thing is orthogonality—then it is easy to produce unit vectors.

To repeat: $Q^{\mathrm{T}}Q = I$ even when Q is rectangular. In that case Q^{T} is only an inverse from the left. For square matrices we also have $QQ^{\mathrm{T}} = I$, so Q^{T} is the two-sided inverse of Q. The rows of a square Q are orthonormal like the columns. ***The inverse is the transpose***. In this square case we call Q an ***orthogonal matrix***.[1]

Here are three examples of orthogonal matrices—rotation and permutation and reflection. The quickest test is to check $Q^{\mathrm{T}}Q = I$.

Example 1 **(Rotation)** Q rotates every vector in the plane by the angle θ:

$$Q = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \quad \text{and} \quad Q^{\mathrm{T}} = Q^{-1} = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix}.$$

The columns of Q are orthogonal (take their dot product). They are unit vectors because $\sin^2\theta + \cos^2\theta = 1$. Those columns give an ***orthonormal basis*** for the plane $\mathbf{R}^2$.

The standard basis vectors $\boldsymbol{i}$ and $\boldsymbol{j}$ are rotated through θ (see Figure 4.10a). Q^{-1} rotates vectors back through $-\theta$. It agrees with Q^{T}, because the cosine of $-\theta$ equals the cosine of θ, and $\sin(-\theta) = -\sin\theta$. We have $Q^{\mathrm{T}}Q = I$ and $QQ^{\mathrm{T}} = I$.

Example 2 **(Permutation)** These matrices change the order to (y, z, x) and (y, x):

$$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} y \\ z \\ x \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} y \\ x \end{bmatrix}.$$

All columns of these Q's are unit vectors (their lengths are obviously 1). They are also orthogonal (the 1's appear in different places). *The inverse of a permutation matrix is its transpose*: $Q^{-1} = Q^{\mathrm{T}}$. The inverse puts the components back into their original order:

[1]"Orthonormal matrix" would have been a better name for Q, but it's not used. Any matrix with orthonormal columns has the letter Q. But we only call it an **orthogonal matrix** when it is square.

$$\textbf{Inverse = transpose:} \quad \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{z} \\ \boldsymbol{x} \end{bmatrix} = \begin{bmatrix} \boldsymbol{x} \\ \boldsymbol{y} \\ \boldsymbol{z} \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{x} \end{bmatrix} = \begin{bmatrix} \boldsymbol{x} \\ \boldsymbol{y} \end{bmatrix}.$$

Every permutation matrix is an orthogonal matrix.

Example 3 **(Reflection)** If $\boldsymbol{u}$ is any unit vector, set $Q = I - 2\boldsymbol{u}\boldsymbol{u}^{\mathrm{T}}$. Notice that $\boldsymbol{u}\boldsymbol{u}^{\mathrm{T}}$ is a matrix while $\boldsymbol{u}^{\mathrm{T}}\boldsymbol{u}$ is the number $\|\boldsymbol{u}\|^2 = 1$. Then Q^{T} and Q^{-1} both equal Q:

$$\boxed{Q^{\mathrm{T}} = I - 2\boldsymbol{u}\boldsymbol{u}^{\mathrm{T}} = Q} \quad \text{and} \quad Q^{\mathrm{T}}Q = I - 4\boldsymbol{u}\boldsymbol{u}^{\mathrm{T}} + 4\boldsymbol{u}\boldsymbol{u}^{\mathrm{T}}\boldsymbol{u}\boldsymbol{u}^{\mathrm{T}} = I. \qquad (2)$$

Reflection matrices $I - 2\boldsymbol{u}\boldsymbol{u}^{\mathrm{T}}$ are symmetric and also orthogonal. If you square them, you get the identity matrix: $Q^2 = Q^{\mathrm{T}}Q = I$. Reflecting twice through a mirror brings back the original, like $(-1)^2 = 1$. Notice $\boldsymbol{u}^{\mathrm{T}}\boldsymbol{u} = 1$ inside $4\boldsymbol{u}\boldsymbol{u}^{\mathrm{T}}\boldsymbol{u}\boldsymbol{u}^{\mathrm{T}}$ in equation (2).

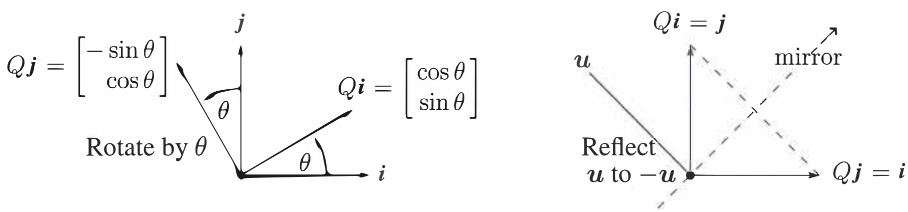


Figure 4.10: Rotation by $Q = \begin{bmatrix} c & -s \\ s & c \end{bmatrix}$ and reflection across 45° by $Q = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$.

As example choose the direction $\boldsymbol{u} = (-1/\sqrt{2}, 1/\sqrt{2})$. Compute $2\boldsymbol{u}\boldsymbol{u}^{\mathrm{T}}$ (column times row) and subtract from I to get the reflection matrix Q in the direction of $\boldsymbol{u}$:

$$\textbf{Reflection} \quad Q = I - 2\begin{bmatrix} .5 & -.5 \\ -.5 & .5 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} y \\ x \end{bmatrix}.$$

When (x, y) goes to (y, x), a vector like $(3, 3)$ doesn't move. It is on the mirror line.

Rotations preserve the length of every vector. So do reflections. So do permutations. So does multiplication by any orthogonal matrix Q—***lengths and angles don't change***.

Proof $\|Q\boldsymbol{x}\|^2$ equals $\|\boldsymbol{x}\|^2$ because $(Q\boldsymbol{x})^{\mathrm{T}}(Q\boldsymbol{x}) = \boldsymbol{x}^{\mathrm{T}}Q^{\mathrm{T}}Q\boldsymbol{x} = \boldsymbol{x}^{\mathrm{T}}I\boldsymbol{x} = \boldsymbol{x}^{\mathrm{T}}\boldsymbol{x}$.

If Q has orthonormal columns ($Q^{\mathrm{T}}Q = I$), it leaves lengths unchanged:

Same length for $Q\boldsymbol{x}$ $\quad$ $\boxed{\|Q\boldsymbol{x}\| = \|\boldsymbol{x}\| \textbf{ for every vector } \boldsymbol{x}.}$ $\qquad$ (3)

Q also preserves dot products: $\boxed{(Q\boldsymbol{x})^{\mathrm{T}}(Q\boldsymbol{y}) = \boldsymbol{x}^{\mathrm{T}}Q^{\mathrm{T}}Q\boldsymbol{y} = \boldsymbol{x}^{\mathrm{T}}\boldsymbol{y}.}$ Just use $Q^{\mathrm{T}}Q = I$!

Projections Using Orthonormal Bases: Q Replaces A

Orthogonal matrices are excellent for computations—numbers can never grow too large when lengths of vectors are fixed. Stable computer codes use Q's as much as possible.

For projections onto subspaces, all formulas involve $A^{\mathrm{T}}A$. The entries of $A^{\mathrm{T}}A$ are the dot products $\boldsymbol{a}_i^{\mathrm{T}}\boldsymbol{a}_j$ of the basis vectors $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_n$.

Suppose the basis vectors are actually orthonormal. The $\boldsymbol{a}$'s become the $\boldsymbol{q}$'s. Then $A^{\mathrm{T}}A$ *simplifies to* $Q^{\mathrm{T}}Q = I$. Look at the improvements in $\widehat{\boldsymbol{x}}$ and $\boldsymbol{p}$ and P. Instead of $Q^{\mathrm{T}}Q$ we print a blank for the identity matrix:

$$\underline{\qquad}\,\widehat{\boldsymbol{x}} = Q^{\mathrm{T}}\boldsymbol{b} \quad \text{and} \quad \boldsymbol{p} = Q\widehat{\boldsymbol{x}} \quad \text{and} \quad P = Q\,\underline{\qquad}\,Q^{\mathrm{T}}. \tag{4}$$

The least squares solution of $Q\boldsymbol{x} = \boldsymbol{b}$ is $\widehat{\boldsymbol{x}} = Q^{\mathrm{T}}\boldsymbol{b}$. The projection matrix is QQ^{T}.

There are no matrices to invert. This is the point of an orthonormal basis. The best $\widehat{\boldsymbol{x}} = Q^{\mathrm{T}}\boldsymbol{b}$ just has dot products of $\boldsymbol{q}_1, \ldots, \boldsymbol{q}_n$ with $\boldsymbol{b}$. We have 1-dimensional projections! The "coupling matrix" or "correlation matrix" $A^{\mathrm{T}}A$ is now $Q^{\mathrm{T}}Q = I$. There is no coupling. When A is Q, with orthonormal columns, here is $\boldsymbol{p} = Q\widehat{\boldsymbol{x}} = QQ^{\mathrm{T}}\boldsymbol{b}$:

Projection onto q's

$$\boldsymbol{p} = \begin{bmatrix} | & & | \\ \boldsymbol{q}_1 & \cdots & \boldsymbol{q}_n \\ | & & | \end{bmatrix} \begin{bmatrix} \boldsymbol{q}_1^{\mathrm{T}}\boldsymbol{b} \\ \vdots \\ \boldsymbol{q}_n^{\mathrm{T}}\boldsymbol{b} \end{bmatrix} = \boldsymbol{q}_1(\boldsymbol{q}_1^{\mathrm{T}}\boldsymbol{b}) + \cdots + \boldsymbol{q}_n(\boldsymbol{q}_n^{\mathrm{T}}\boldsymbol{b}). \tag{5}$$

Important case: When Q is square and $m = n$, the subspace is the whole space. Then $Q^{\mathrm{T}} = Q^{-1}$ and $\widehat{\boldsymbol{x}} = Q^{\mathrm{T}}\boldsymbol{b}$ is the same as $\boldsymbol{x} = Q^{-1}\boldsymbol{b}$. The solution is exact! The projection of $\boldsymbol{b}$ onto the whole space is $\boldsymbol{b}$ itself. In this case $\boldsymbol{p} = \boldsymbol{b}$ and $P = QQ^{\mathrm{T}} = I$.

You may think that projection onto the whole space is not worth mentioning. But when $\boldsymbol{p} = \boldsymbol{b}$, our formula assembles $\boldsymbol{b}$ out of its 1-dimensional projections. If $\boldsymbol{q}_1, \ldots, \boldsymbol{q}_n$ is an orthonormal basis for the whole space, then Q is square. Every $\boldsymbol{b} = QQ^{\mathrm{T}}\boldsymbol{b}$ *is the sum of its components along the* $\boldsymbol{q}$'s:

$$\boldsymbol{b} = \boldsymbol{q}_1(\boldsymbol{q}_1^{\mathrm{T}}\boldsymbol{b}) + \boldsymbol{q}_2(\boldsymbol{q}_2^{\mathrm{T}}\boldsymbol{b}) + \cdots + \boldsymbol{q}_n(\boldsymbol{q}_n^{\mathrm{T}}\boldsymbol{b}). \tag{6}$$

Transforms $QQ^{\mathrm{T}} = I$ is the foundation of Fourier series and all the great "transforms" of applied mathematics. They break vectors $\boldsymbol{b}$ or functions $f(x)$ into perpendicular pieces. Then by adding the pieces in (6), the inverse transform puts $\boldsymbol{b}$ and $f(x)$ back together.

Example 4 The columns of this orthogonal Q are orthonormal vectors $\boldsymbol{q}_1, \boldsymbol{q}_2, \boldsymbol{q}_3$:

$$\boldsymbol{m = n = 3} \qquad Q = \frac{1}{3}\begin{bmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{bmatrix} \quad \text{has} \quad \boldsymbol{Q^{\mathrm{T}}Q = QQ^{\mathrm{T}} = I}.$$

The separate projections of $\boldsymbol{b} = (0,0,1)$ onto $\boldsymbol{q}_1$ and $\boldsymbol{q}_2$ and $\boldsymbol{q}_3$ are $\boldsymbol{p}_1$ and $\boldsymbol{p}_2$ and $\boldsymbol{p}_3$:

$$\boldsymbol{q}_1(\boldsymbol{q}_1^{\mathrm{T}}\boldsymbol{b}) = \tfrac{2}{3}\boldsymbol{q}_1 \quad \text{and} \quad \boldsymbol{q}_2(\boldsymbol{q}_2^{\mathrm{T}}\boldsymbol{b}) = \tfrac{2}{3}\boldsymbol{q}_2 \quad \text{and} \quad \boldsymbol{q}_3(\boldsymbol{q}_3^{\mathrm{T}}\boldsymbol{b}) = -\tfrac{1}{3}\boldsymbol{q}_3.$$

The sum of the first two is the projection of $\boldsymbol{b}$ onto the *plane* of $\boldsymbol{q}_1$ and $\boldsymbol{q}_2$. The sum of all three is the projection of $\boldsymbol{b}$ onto the *whole space*—which is $\boldsymbol{p}_1 + \boldsymbol{p}_2 + \boldsymbol{p}_3 = \boldsymbol{b}$ itself:

Reconstruct b
$b = p_1 + p_2 + p_3$

$$\frac{2}{3}q_1 + \frac{2}{3}q_2 - \frac{1}{3}q_3 = \frac{1}{9}\begin{bmatrix} -2+4-2 \\ 4-2-2 \\ 4+4+1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = b.$$

The Gram-Schmidt Process

The point of this section is that "orthogonal is good". Projections and least squares always involve $A^{\mathrm{T}}A$. When this matrix becomes $Q^{\mathrm{T}}Q = I$, the inverse is no problem. The one-dimensional projections are uncoupled. The best $\widehat{\boldsymbol{x}}$ is $Q^{\mathrm{T}}\boldsymbol{b}$ (just n separate dot products). For this to be true, we had to say "*If* the vectors are orthonormal". ***Now we explain the "Gram-Schmidt way" to create orthonormal vectors.***

Start with three independent vectors $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$. We intend to construct three orthogonal vectors $\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}$. Then (at the end may be easiest) we divide $\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}$ by their lengths. That produces three orthonormal vectors $\boldsymbol{q}_1 = \boldsymbol{A}/\|\boldsymbol{A}\|$, $\boldsymbol{q}_2 = \boldsymbol{B}/\|\boldsymbol{B}\|$, $\boldsymbol{q}_3 = \boldsymbol{C}/\|\boldsymbol{C}\|$.

Gram-Schmidt Begin by choosing $\boldsymbol{A} = \boldsymbol{a}$. This first direction is accepted as it comes. The next direction $\boldsymbol{B}$ must be perpendicular to $\boldsymbol{A}$. ***Start with $\boldsymbol{b}$ and subtract its projection along $\boldsymbol{A}$***. This leaves the perpendicular part, which is the orthogonal vector $\boldsymbol{B}$:

First Gram-Schmidt step
$$\boxed{B = b - \frac{A^{\mathrm{T}}b}{A^{\mathrm{T}}A}A.} \qquad (7)$$

$\boldsymbol{A}$ and $\boldsymbol{B}$ are orthogonal in Figure 4.11. Multiply equation (7) by $\boldsymbol{A}^{\mathrm{T}}$ to verify that $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{B} = \boldsymbol{A}^{\mathrm{T}}\boldsymbol{b} - \boldsymbol{A}^{\mathrm{T}}\boldsymbol{b} = 0$. This vector $\boldsymbol{B}$ is what we have called the error vector $\boldsymbol{e}$, perpendicular to $\boldsymbol{A}$. Notice that $\boldsymbol{B}$ in equation (7) is not zero (otherwise $\boldsymbol{a}$ and $\boldsymbol{b}$ would be dependent). The directions $\boldsymbol{A}$ and $\boldsymbol{B}$ are now set.

The third direction starts with $\boldsymbol{c}$. This is not a combination of $\boldsymbol{A}$ and $\boldsymbol{B}$ (because $\boldsymbol{c}$ is not a combination of $\boldsymbol{a}$ and $\boldsymbol{b}$). But most likely $\boldsymbol{c}$ is not perpendicular to $\boldsymbol{A}$ and $\boldsymbol{B}$. So subtract off its components in those two directions to get a perpendicular direction $\boldsymbol{C}$:

Next Gram-Schmidt step
$$\boxed{C = c - \frac{A^{\mathrm{T}}c}{A^{\mathrm{T}}A}A - \frac{B^{\mathrm{T}}c}{B^{\mathrm{T}}B}B.} \qquad (8)$$

This is the one and only idea of the Gram-Schmidt process. ***Subtract from every new vector its projections in the directions already set.*** That idea is repeated at every step.[2] If we had a fourth vector $\boldsymbol{d}$, we would subtract three projections onto $\boldsymbol{A}$, $\boldsymbol{B}, \boldsymbol{C}$ to get $\boldsymbol{D}$.

[2] I think Gram had the idea. I don't really know where Schmidt came in.

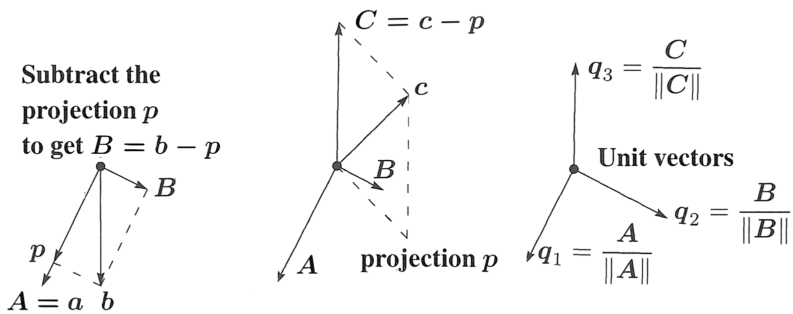


Figure 4.11: First project b onto the line through a and find the orthogonal B as $b - p$. Then project c onto the AB plane and find C as $c - p$. Divide by $\|A\|$, $\|B\|$, $\|C\|$.

At the end, *or immediately when each one is found*, divide the orthogonal vectors A, B, C, D by their lengths. The resulting vectors q_1, q_2, q_3, q_4 are orthonormal.

Example of **Gram-Schmidt** Suppose the independent non-orthogonal vectors a, b, c are

$$a = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix} \quad \text{and} \quad b = \begin{bmatrix} 2 \\ 0 \\ -2 \end{bmatrix} \quad \text{and} \quad c = \begin{bmatrix} 3 \\ -3 \\ 3 \end{bmatrix}.$$

Then $A = a$ has $A^{\mathrm{T}}A = 2$ and $A^{\mathrm{T}}b = 2$. Subtract from b its projection p along A:

First step $$B = b - \frac{A^{\mathrm{T}}b}{A^{\mathrm{T}}A}A = b - \frac{2}{2}A = \begin{bmatrix} 1 \\ 1 \\ -2 \end{bmatrix}.$$

Check: $A^{\mathrm{T}}B = 0$ as required. Now subtract the projections of c on A and B to get C:

Next step $$C = c - \frac{A^{\mathrm{T}}c}{A^{\mathrm{T}}A}A - \frac{B^{\mathrm{T}}c}{B^{\mathrm{T}}B}B = c - \frac{6}{2}A + \frac{6}{6}B = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}.$$

Check: $C = (1, 1, 1)$ is perpendicular to both A and B. Finally convert A, B, C to unit vectors (length 1, orthonormal). The lengths of A, B, C are $\sqrt{2}$ and $\sqrt{6}$ and $\sqrt{3}$. Divide by those lengths, for an orthonormal basis:

$$q_1 = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix} \quad \text{and} \quad q_2 = \frac{1}{\sqrt{6}}\begin{bmatrix} 1 \\ 1 \\ -2 \end{bmatrix} \quad \text{and} \quad q_3 = \frac{1}{\sqrt{3}}\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}.$$

Usually A, B, C contain fractions. Almost always q_1, q_2, q_3 contain square roots.

The Factorization $A = QR$

We started with a matrix A, whose columns were $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$. We ended with a matrix Q, whose columns are $\boldsymbol{q}_1, \boldsymbol{q}_2, \boldsymbol{q}_3$. How are those matrices related? Since the vectors $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$ are combinations of the $\boldsymbol{q}$'s (and vice versa), there must be a third matrix connecting A to Q. This third matrix is the triangular R in $A = QR$.

The first step was $\boldsymbol{q}_1 = \boldsymbol{a}/\|\boldsymbol{a}\|$ (other vectors not involved). The second step was equation (7), where $\boldsymbol{b}$ is a combination of $\boldsymbol{A}$ and $\boldsymbol{B}$. At that stage $\boldsymbol{C}$ and $\boldsymbol{q}_3$ were not involved. This non-involvement of later vectors is the key point of Gram-Schmidt:

- The vectors $\boldsymbol{a}$ and $\boldsymbol{A}$ and $\boldsymbol{q}_1$ are all along a single line.
- The vectors $\boldsymbol{a}, \boldsymbol{b}$ and $\boldsymbol{A}, \boldsymbol{B}$ and $\boldsymbol{q}_1, \boldsymbol{q}_2$ are all in the same plane.
- The vectors $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$ and $\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}$ and $\boldsymbol{q}_1, \boldsymbol{q}_2, \boldsymbol{q}_3$ are in one subspace (dimension 3).

At every step $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_k$ are combinations of $\boldsymbol{q}_1, \ldots, \boldsymbol{q}_k$. Later $\boldsymbol{q}$'s are not involved. The connecting matrix R is ***triangular***, and we have $A = QR$:

$$\begin{bmatrix} & & \\ \boldsymbol{a} & \boldsymbol{b} & \boldsymbol{c} \\ & & \end{bmatrix} = \begin{bmatrix} & & \\ \boldsymbol{q}_1 & \boldsymbol{q}_2 & \boldsymbol{q}_3 \\ & & \end{bmatrix} \begin{bmatrix} \boldsymbol{q}_1^{\mathrm{T}}\boldsymbol{a} & \boldsymbol{q}_1^{\mathrm{T}}\boldsymbol{b} & \boldsymbol{q}_1^{\mathrm{T}}\boldsymbol{c} \\ & \boldsymbol{q}_2^{\mathrm{T}}\boldsymbol{b} & \boldsymbol{q}_2^{\mathrm{T}}\boldsymbol{c} \\ & & \boldsymbol{q}_3^{\mathrm{T}}\boldsymbol{c} \end{bmatrix} \quad \text{or} \quad \boldsymbol{A = QR}. \tag{9}$$

$A = QR$ is Gram-Schmidt in a nutshell. Multiply by Q^{T} to recognize $\boldsymbol{R} = \boldsymbol{Q}^{\mathrm{T}}\boldsymbol{A}$ above.

(Gram-Schmidt) From independent vectors $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_n$, Gram-Schmidt constructs orthonormal vectors $\boldsymbol{q}_1, \ldots, \boldsymbol{q}_n$. The matrices with these columns satisfy $A = QR$. Then $R = Q^{\mathrm{T}}A$ is ***upper triangular*** because later $\boldsymbol{q}$'s are orthogonal to earlier $\boldsymbol{a}$'s.

Here are the original $\boldsymbol{a}$'s and the final $\boldsymbol{q}$'s from the example. The i, j entry of $R = Q^{\mathrm{T}}A$ is row i of Q^{T} times column j of A. The dot products $\boldsymbol{q}_i^{\mathrm{T}}\boldsymbol{a}_j$ go into R. **Then $\boldsymbol{A = QR}$:**

$$A = \begin{bmatrix} 1 & 2 & 3 \\ -1 & 0 & -3 \\ 0 & -2 & 3 \end{bmatrix} = \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{6} & 1/\sqrt{3} \\ -1/\sqrt{2} & 1/\sqrt{6} & 1/\sqrt{3} \\ 0 & -2/\sqrt{6} & 1/\sqrt{3} \end{bmatrix} \begin{bmatrix} \sqrt{\mathbf{2}} & \sqrt{2} & \sqrt{18} \\ \mathbf{0} & \sqrt{\mathbf{6}} & -\sqrt{6} \\ \mathbf{0} & \mathbf{0} & \sqrt{\mathbf{3}} \end{bmatrix} = QR.$$

Look closely at Q and R. The lengths of $\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}$ are $\sqrt{2}, \sqrt{6}, \sqrt{3}$ on the diagonal of R. The columns of Q are orthonormal. Because of the square roots, QR might look harder than LU. Both factorizations are absolutely central to calculations in linear algebra.

Any m by n matrix A with independent columns can be factored into $A = QR$. The m by n matrix Q has orthonormal columns, and the square matrix R is upper triangular with positive diagonal. We must not forget why this is useful for least squares: $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A} = (\boldsymbol{QR})^{\mathrm{T}}\boldsymbol{QR} = \boldsymbol{R}^{\mathrm{T}}\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{QR} = \boldsymbol{R}^{\mathrm{T}}\boldsymbol{R}$. The least squares equation $A^{\mathrm{T}}A\widehat{\boldsymbol{x}} = A^{\mathrm{T}}\boldsymbol{b}$ simplifies to $R^{\mathrm{T}}R\widehat{\boldsymbol{x}} = R^{\mathrm{T}}Q^{\mathrm{T}}\boldsymbol{b}$. Then finally we reach $R\widehat{\boldsymbol{x}} = Q^{\mathrm{T}}\boldsymbol{b}$: good.

$$\textbf{Least squares} \qquad R^{\mathrm{T}}R\widehat{\boldsymbol{x}} = R^{\mathrm{T}}Q^{\mathrm{T}}\boldsymbol{b} \ \text{ or } \ R\widehat{\boldsymbol{x}} = Q^{\mathrm{T}}\boldsymbol{b} \ \text{ or } \ \boxed{\widehat{\boldsymbol{x}} = R^{-1}Q^{\mathrm{T}}\boldsymbol{b}} \qquad (10)$$

Instead of solving $A\boldsymbol{x} = \boldsymbol{b}$, which is impossible, we solve $R\widehat{\boldsymbol{x}} = Q^{\mathrm{T}}\boldsymbol{b}$ by back substitution—which is very fast. The real cost is the mn^2 multiplications in the Gram-Schmidt process, which are needed to construct the orthogonal Q and the triangular R with $A = QR$.

Below is an informal code. It executes equations (11) for $j = 1$ then $j = 2$ and eventually $j = n$. The important lines 4-5 subtract from $\boldsymbol{v} = \boldsymbol{a}_j$ its projection onto each $\boldsymbol{q}_i, i < j$. The last line of that code normalizes $\boldsymbol{v}$ (divides by $r_{jj} = ||\boldsymbol{v}||$) to get the unit vector $\boldsymbol{q}_j$:

$$r_{kj} = \sum_{i=1}^{m} q_{ik}v_{ij} \ \text{ and } \ v_{ij} = v_{ij} - q_{ik}r_{kj} \ \text{ and } \ r_{jj} = \left(\sum_{i=1}^{m} v_{ij}^2\right)^{1/2} \ \text{ and } \ q_{ij} = \frac{v_{ij}}{r_{jj}}. \qquad (11)$$

Starting from $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c} = \boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3$ this code will construct $\boldsymbol{q}_1$, then $\boldsymbol{B}$, $\boldsymbol{q}_2$, then $\boldsymbol{C}$, $\boldsymbol{q}_3$:

$$\boldsymbol{q}_1 = \boldsymbol{a}_1/\|\boldsymbol{a}_1\| \qquad \boldsymbol{B} = \boldsymbol{a}_2 - (\boldsymbol{q}_1^{\mathrm{T}}\boldsymbol{a}_2)\boldsymbol{q}_1 \qquad \boldsymbol{q}_2 = \boldsymbol{B}/\|\boldsymbol{B}\|$$

$$\boldsymbol{C}^* = \boldsymbol{a}_3 - (\boldsymbol{q}_1^{\mathrm{T}}\boldsymbol{a}_3)\boldsymbol{q}_1 \qquad \boldsymbol{C} = \boldsymbol{C}^* - (\boldsymbol{q}_2^{\mathrm{T}}\boldsymbol{C}^*)\boldsymbol{q}_2 \qquad \boldsymbol{q}_3 = \boldsymbol{C}/\|\boldsymbol{C}\|$$

Equation (11) subtracts **one projection at a time** as in $\boldsymbol{C}^*$ and $\boldsymbol{C}$. That change is called ***modified Gram-Schmidt***. This code is numerically more stable than equation (8) which subtracts all projections at once.

```
for j = 1:n                       % modified Gram-Schmidt
  v = A(:, j);                    % v begins as column j of the original A
  for i = 1:j-1                   % columns q_1 to q_{j-1} are already settled in Q
    R(i, j) = Q(:, i)'*v;         % compute R_ij = q_i^T a_j which is q_i^T v
    v = v-R(i, j)*Q(:, i);        % subtract the projection (q_i^T v) q_i
  end                             % v is now perpendicular to all of q_1, ..., q_{j-1}
  R(j, j) = norm(v);              % the diagonal entries R_jj are lengths
  Q(:, j) = v/R(j, j);            % divide v by its length to get the next q_j
end                               % the "for j = 1 : n loop" produces all of the q_j
```

To recover column j of A, undo the last step and the middle steps of the code:

$$R(j,j)\boldsymbol{q}_j = (\boldsymbol{v} \textit{ minus its projections}) = (\text{column } j \text{ of } A) - \sum_{i=1}^{j-1} R(i,j)\boldsymbol{q}_i\,. \qquad (12)$$

Moving the sum to the far left, this is column j in the multiplication $QR = A$.

Confession Good software like LAPACK, used in good systems like MATLAB and Julia and Python, will not use this Gram-Schmidt code. There is now a better way. "Householder reflections" act on A to produce the upper triangular R. This happens one column at a time in the same way that elimination produces the upper triangular U in LU.

Those reflection matrices $I - 2\boldsymbol{u}\boldsymbol{u}^{\mathrm{T}}$ will be described in Chapter 11 on numerical linear algebra. If A is tridiagonal we can simplify even more to use 2 by 2 rotations. The result is always $A = QR$ and the MATLAB command to orthogonalize A is $[Q, R] = \mathrm{qr}(A)$. I believe that Gram-Schmidt is still the good process to understand, even if the reflections or rotations lead to a more perfect Q.

■ REVIEW OF THE KEY IDEAS ■

1. If the orthonormal vectors $\boldsymbol{q}_1, \ldots, \boldsymbol{q}_n$ are the columns of Q, then $\boldsymbol{q}_i^{\mathrm{T}}\boldsymbol{q}_j = 0$ and $\boldsymbol{q}_i^{\mathrm{T}}\boldsymbol{q}_i = 1$ translate into the matrix multiplication $Q^{\mathrm{T}}Q = I$.
2. If Q is square (an ***orthogonal matrix***) then $Q^{\mathrm{T}} = Q^{-1}$: ***transpose*** $=$ ***inverse***.
3. The length of $Q\boldsymbol{x}$ equals the length of $\boldsymbol{x}$: $\|Q\boldsymbol{x}\| = \|\boldsymbol{x}\|$.
4. The projection onto the column space of Q spanned by the $\boldsymbol{q}$'s is $P = QQ^{\mathrm{T}}$.
5. If Q is square then $P = QQ^{\mathrm{T}} = I$ and every $\boldsymbol{b} = \boldsymbol{q}_1(\boldsymbol{q}_1^{\mathrm{T}}\boldsymbol{b}) + \cdots + \boldsymbol{q}_n(\boldsymbol{q}_n^{\mathrm{T}}\boldsymbol{b})$.
6. Gram-Schmidt produces orthonormal vectors $\boldsymbol{q}_1, \boldsymbol{q}_2, \boldsymbol{q}_3$ from independent $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$. In matrix form this is the factorization $A = QR = (\text{orthogonal } Q)(\text{triangular } R)$.

■ WORKED EXAMPLES ■

4.4 A Add two more columns with all entries 1 or -1, so the columns of this 4 by 4 "Hadamard matrix" are orthogonal. How do you turn H_4 into an *orthogonal matrix* Q?

$$H_2 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \qquad H_4 = \begin{bmatrix} 1 & 1 & x & x \\ 1 & -1 & x & x \\ 1 & 1 & x & x \\ 1 & -1 & x & x \end{bmatrix} \qquad \text{and} \qquad Q_4 = \begin{bmatrix} \quad & \quad & \quad & \quad \\ & & & \\ & & & \\ & & & \end{bmatrix}$$

The block matrix $H_8 = \begin{bmatrix} H_4 & H_4 \\ H_4 & -H_4 \end{bmatrix}$ is the next Hadamard matrix with 1's and -1's. What is the product $H_8^{\mathrm{T}} H_8$?

The projection of $\boldsymbol{b} = (6, 0, 0, 2)$ onto the first column of H_4 is $\boldsymbol{p}_1 = (2, 2, 2, 2)$. The projection onto the second column is $\boldsymbol{p}_2 = (1, -1, 1, -1)$. What is the projection $\boldsymbol{p}_{1,2}$ of $\boldsymbol{b}$ onto the 2-dimensional space spanned by the first two columns?

Solution H_4 can be built from H_2 just as H_8 is built from H_4:

$$H_4 = \begin{bmatrix} H_2 & H_2 \\ H_2 & -H_2 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix} \text{ has orthogonal columns.}$$

Then $Q = H/2$ has orthonormal columns. Dividing by 2 gives unit vectors in Q. A 5 by 5 Hadamard matrix is impossible because the dot product of columns would have five 1's and/or -1's and could not add to zero. H_8 has orthogonal columns of length $\sqrt{8}$.

$$H_8^{\mathrm{T}} H_8 = \begin{bmatrix} H^{\mathrm{T}} & H^{\mathrm{T}} \\ H^{\mathrm{T}} & -H^{\mathrm{T}} \end{bmatrix} \begin{bmatrix} H & H \\ H & -H \end{bmatrix} = \begin{bmatrix} 2H^{\mathrm{T}}H & 0 \\ 0 & 2H^{\mathrm{T}}H \end{bmatrix} = \begin{bmatrix} 8I & 0 \\ 0 & 8I \end{bmatrix}. \; Q_8 = \frac{H_8}{\sqrt{8}}$$

4.4 B What is the key point of orthogonal columns? Answer: $A^{\mathrm{T}}A$ is diagonal and easy to invert. **We can project onto lines and just add**. The axes are orthogonal.

Add p's Projection $\boldsymbol{p}_{1,2}$ onto a plane equals $\boldsymbol{p}_1 + \boldsymbol{p}_2$ onto orthogonal lines.

Problem Set 4.4

Problems 1–12 are about orthogonal vectors and orthogonal matrices.

1 Are these pairs of vectors orthonormal or only orthogonal or only independent?

(a) $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $\begin{bmatrix} -1 \\ 1 \end{bmatrix}$ (b) $\begin{bmatrix} .6 \\ .8 \end{bmatrix}$ and $\begin{bmatrix} .4 \\ -.3 \end{bmatrix}$ (c) $\begin{bmatrix} \cos\theta \\ \sin\theta \end{bmatrix}$ and $\begin{bmatrix} -\sin\theta \\ \cos\theta \end{bmatrix}$.

Change the second vector when necessary to produce orthonormal vectors.

2 The vectors $(2, 2, -1)$ and $(-1, 2, 2)$ are orthogonal. Divide them by their lengths to find orthonormal vectors $\boldsymbol{q}_1$ and $\boldsymbol{q}_2$. Put those into the columns of Q and multiply $Q^{\mathrm{T}}Q$ and QQ^{T}.

3 (a) If A has three orthogonal columns each of length 4, what is $A^{\mathrm{T}}A$?

(b) If A has three orthogonal columns of lengths $1, 2, 3$, what is $A^{\mathrm{T}}A$?

4 Give an example of each of the following:

(a) A matrix Q that has orthonormal columns but $QQ^{\mathrm{T}} \neq I$.

(b) Two orthogonal vectors that are not linearly independent.

(c) An orthonormal basis for $\mathbf{R}^3$, including the vector $\boldsymbol{q}_1 = (1, 1, 1)/\sqrt{3}$.

5 Find two orthogonal vectors in the plane $x + y + 2z = 0$. Make them orthonormal.

6 If Q_1 and Q_2 are orthogonal matrices, show that their product Q_1Q_2 is also an orthogonal matrix. (Use $Q^{\mathrm{T}}Q = I$.)

7 If Q has orthonormal columns, what is the least squares solution $\widehat{\boldsymbol{x}}$ to $Q\boldsymbol{x} = \boldsymbol{b}$?

8 If $\boldsymbol{q}_1$ and $\boldsymbol{q}_2$ are orthonormal vectors in $\mathbf{R}^5$, what combination ____ $q_1 +$ ____ q_2 is closest to a given vector $\boldsymbol{b}$?

9 (a) Compute $P = QQ^{\mathrm{T}}$ when $\boldsymbol{q}_1 = (.8, .6, 0)$ and $\boldsymbol{q}_2 = (-.6, .8, 0)$. Verify that $P^2 = P$.

(b) Prove that always $(QQ^{\mathrm{T}})^2 = QQ^{\mathrm{T}}$ by using $Q^{\mathrm{T}}Q = I$. Then $P = QQ^{\mathrm{T}}$ is the projection matrix onto the column space of Q.

10 Orthonormal vectors are automatically linearly independent.

(a) Vector proof: When $c_1\boldsymbol{q}_1 + c_2\boldsymbol{q}_2 + c_3\boldsymbol{q}_3 = \mathbf{0}$, what dot product leads to $c_1 = 0$? Similarly $c_2 = 0$ and $c_3 = 0$. Thus the $\boldsymbol{q}$'s are independent.

(b) Matrix proof: Show that $Q\boldsymbol{x} = \mathbf{0}$ leads to $\boldsymbol{x} = \mathbf{0}$. Since Q may be rectangular, you can use Q^{T} but not Q^{-1}.

11 (a) Gram-Schmidt: Find orthonormal vectors $\boldsymbol{q}_1$ and $\boldsymbol{q}_2$ in the plane spanned by $\boldsymbol{a} = (1, 3, 4, 5, 7)$ and $\boldsymbol{b} = (-6, 6, 8, 0, 8)$.

(b) Which vector in this plane is closest to $(1, 0, 0, 0, 0)$?

12 If $\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3$ is a basis for $\mathbf{R}^3$, any vector $\boldsymbol{b}$ can be written as

$$\boldsymbol{b} = x_1\boldsymbol{a}_1 + x_2\boldsymbol{a}_2 + x_3\boldsymbol{a}_3 \qquad \text{or} \qquad \begin{bmatrix} & & \\ \boldsymbol{a}_1 & \boldsymbol{a}_2 & \boldsymbol{a}_3 \\ & & \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \boldsymbol{b}.$$

(a) Suppose the $\boldsymbol{a}$'s are orthonormal. Show that $x_1 = \boldsymbol{a}_1^{\mathrm{T}}\boldsymbol{b}$.

(b) Suppose the $\boldsymbol{a}$'s are orthogonal. Show that $x_1 = \boldsymbol{a}_1^{\mathrm{T}}\boldsymbol{b}/\boldsymbol{a}_1^{\mathrm{T}}\boldsymbol{a}_1$.

(c) If the $\boldsymbol{a}$'s are independent, x_1 is the first component of ____ times $\boldsymbol{b}$.

Problems 13–25 are about the Gram-Schmidt process and $A = QR$.

13 What multiple of $\boldsymbol{a} = \left[\begin{smallmatrix} 1 \\ 1 \end{smallmatrix}\right]$ should be subtracted from $\boldsymbol{b} = \left[\begin{smallmatrix} 4 \\ 0 \end{smallmatrix}\right]$ to make the result $\boldsymbol{B}$ orthogonal to $\boldsymbol{a}$? Sketch a figure to show $\boldsymbol{a}, \boldsymbol{b}$, and $\boldsymbol{B}$.

14 Complete the Gram-Schmidt process in Problem 13 by computing $\boldsymbol{q}_1 = \boldsymbol{a}/\|\boldsymbol{a}\|$ and $\boldsymbol{q}_2 = \boldsymbol{B}/\|\boldsymbol{B}\|$ and factoring into QR:

$$\begin{bmatrix} 1 & 4 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} \boldsymbol{q}_1 & \boldsymbol{q}_2 \end{bmatrix} \begin{bmatrix} \|\boldsymbol{a}\| & ? \\ 0 & \|\boldsymbol{B}\| \end{bmatrix}.$$

15 (a) Find orthonormal vectors $\boldsymbol{q}_1, \boldsymbol{q}_2, \boldsymbol{q}_3$ such that $\boldsymbol{q}_1, \boldsymbol{q}_2$ span the column space of

$$A = \begin{bmatrix} 1 & 1 \\ 2 & -1 \\ -2 & 4 \end{bmatrix}.$$

(b) Which of the four fundamental subspaces contains $\boldsymbol{q}_3$?

(c) Solve $A\boldsymbol{x} = (1, 2, 7)$ by least squares.

16 What multiple of $\boldsymbol{a} = (4, 5, 2, 2)$ is closest to $\boldsymbol{b} = (1, 2, 0, 0)$? Find orthonormal vectors $\boldsymbol{q}_1$ and $\boldsymbol{q}_2$ in the plane of $\boldsymbol{a}$ and $\boldsymbol{b}$.

17 Find the projection of $\boldsymbol{b}$ onto the line through $\boldsymbol{a}$:

$$\boldsymbol{a} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \quad \text{and} \quad \boldsymbol{b} = \begin{bmatrix} 1 \\ 3 \\ 5 \end{bmatrix} \quad \text{and} \quad \boldsymbol{p} = ? \quad \text{and} \quad \boldsymbol{e} = \boldsymbol{b} - \boldsymbol{p} = ?$$

Compute the orthonormal vectors $\boldsymbol{q}_1 = \boldsymbol{a}/\|\boldsymbol{a}\|$ and $\boldsymbol{q}_2 = \boldsymbol{e}/\|\boldsymbol{e}\|$.

18 (Recommended) Find orthogonal vectors $\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}$ by Gram-Schmidt from $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$:

$$\boldsymbol{a} = (1, -1, 0, 0) \qquad \boldsymbol{b} = (0, 1, -1, 0) \qquad \boldsymbol{c} = (0, 0, 1, -1).$$

$\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}$ and $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$ are bases for the vectors perpendicular to $\boldsymbol{d} = (1, 1, 1, 1)$.

19 If $A = QR$ then $A^{\mathrm{T}}A = R^{\mathrm{T}}R =$ _____ triangular times _____ triangular. *Gram-Schmidt on A corresponds to elimination on $A^{\mathrm{T}}A$.* The pivots for $A^{\mathrm{T}}A$ must be the squares of diagonal entries of R. Find Q and R by Gram-Schmidt for this A:

$$A = \begin{bmatrix} -1 & 1 \\ 2 & 1 \\ 2 & 4 \end{bmatrix} \quad \text{and} \quad A^{\mathrm{T}}A = \begin{bmatrix} 9 & 9 \\ 9 & 18 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 9 & \\ & 9 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}.$$

20 True or false (give an example in either case):

(a) Q^{-1} is an orthogonal matrix when Q is an orthogonal matrix.

(b) If Q (3 by 2) has orthonormal columns then $\|Q\boldsymbol{x}\|$ always equals $\|\boldsymbol{x}\|$.

21 Find an orthonormal basis for the column space of A:

$$A = \begin{bmatrix} 1 & -2 \\ 1 & 0 \\ 1 & 1 \\ 1 & 3 \end{bmatrix} \quad \text{and} \quad \boldsymbol{b} = \begin{bmatrix} -4 \\ -3 \\ 3 \\ 0 \end{bmatrix}.$$

Then compute the projection of $\boldsymbol{b}$ onto that column space.

22 Find orthogonal vectors $\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}$ by Gram-Schmidt from

$$\boldsymbol{a} = \begin{bmatrix} 1 \\ 1 \\ 2 \end{bmatrix} \quad \text{and} \quad \boldsymbol{b} = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix} \quad \text{and} \quad \boldsymbol{c} = \begin{bmatrix} 1 \\ 0 \\ 4 \end{bmatrix}.$$

23 Find $\boldsymbol{q}_1, \boldsymbol{q}_2, \boldsymbol{q}_3$ (orthonormal) as combinations of $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$ (independent columns). Then write A as QR:

$$A = \begin{bmatrix} 1 & 2 & 4 \\ 0 & 0 & 5 \\ 0 & 3 & 6 \end{bmatrix}.$$

24 (a) Find a basis for the subspace $\boldsymbol{S}$ in $\mathbf{R}^4$ spanned by all solutions of

$$x_1 + x_2 + x_3 - x_4 = 0.$$

(b) Find a basis for the orthogonal complement $\boldsymbol{S}^{\perp}$.

(c) Find $\boldsymbol{b}_1$ in $\boldsymbol{S}$ and $\boldsymbol{b}_2$ in $\boldsymbol{S}^{\perp}$ so that $\boldsymbol{b}_1 + \boldsymbol{b}_2 = \boldsymbol{b} = (1, 1, 1, 1)$.

25 If $ad - bc > 0$, the entries in $A = QR$ are

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} = \frac{\begin{bmatrix} a & -c \\ c & a \end{bmatrix}}{\sqrt{a^2 + c^2}} \frac{\begin{bmatrix} a^2 + c^2 & ab + cd \\ 0 & ad - bc \end{bmatrix}}{\sqrt{a^2 + c^2}}.$$

Write $A = QR$ when $a, b, c, d = 2, 1, 1, 1$ and also $1, 1, 1, 1$. Which entry of R becomes zero when the columns are dependent and Gram-Schmidt breaks down?

Problems 26–29 use the QR code in equation (11). It executes Gram-Schmidt.

26 Show why $\boldsymbol{C}$ (found via $\boldsymbol{C}^*$ in the steps after (11)) is equal to $\boldsymbol{C}$ in equation (8).

27 Equation (8) subtracts from $\boldsymbol{c}$ its components along $\boldsymbol{A}$ and $\boldsymbol{B}$. Why not subtract the components along $\boldsymbol{a}$ and along $\boldsymbol{b}$?

28 Where are the mn^2 multiplications in equation (11)?

29 Apply the MATLAB qr code to $\boldsymbol{a} = (2, 2, -1)$, $\boldsymbol{b} = (0, -3, 3)$, $\boldsymbol{c} = (1, 0, 0)$. What are the $\boldsymbol{q}$'s?

Problems 30–35 involve orthogonal matrices that are special.

30 The first four ***wavelets*** are in the columns of this wavelet matrix W:

$$W = \frac{1}{2} \begin{bmatrix} 1 & 1 & \sqrt{2} & 0 \\ 1 & 1 & -\sqrt{2} & 0 \\ 1 & -1 & 0 & \sqrt{2} \\ 1 & -1 & 0 & -\sqrt{2} \end{bmatrix}.$$

What is special about the columns? Find the inverse wavelet transform W^{-1}.

31 (a) Choose c so that Q is an orthogonal matrix:

$$Q = c \begin{bmatrix} 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 \\ -1 & -1 & -1 & 1 \end{bmatrix}.$$

Project $\boldsymbol{b} = (1, 1, 1, 1)$ onto the first column. Then project $\boldsymbol{b}$ onto the plane of the first two columns.

32 If $\boldsymbol{u}$ is a unit vector, then $Q = I - 2\boldsymbol{u}\boldsymbol{u}^{\mathrm{T}}$ is a reflection matrix (Example 3). Find Q_1 from $\boldsymbol{u} = (0, 1)$ and Q_2 from $\boldsymbol{u} = (0, \sqrt{2}/2, \sqrt{2}/2)$. Draw the reflections when Q_1 and Q_2 multiply the vectors $(1, 2)$ and $(1, 1, 1)$.

33 Find all matrices that are both orthogonal and lower triangular.

34 $Q = I - 2\boldsymbol{u}\boldsymbol{u}^{\mathrm{T}}$ is a reflection matrix when $\boldsymbol{u}^{\mathrm{T}}\boldsymbol{u} = 1$. Two reflections give $Q^2 = I$.

(a) Show that $Q\boldsymbol{u} = -\boldsymbol{u}$. The mirror is perpendicular to $\boldsymbol{u}$.

(b) Find $Q\boldsymbol{v}$ when $\boldsymbol{u}^{\mathrm{T}}\boldsymbol{v} = 0$. The mirror contains $\boldsymbol{v}$. It reflects to itself.

Challenge Problems

35 (MATLAB) Factor $[Q, R] = \mathbf{qr}(A)$ for $A = \mathbf{eye}(4) - \mathbf{diag}([1\ \ 1\ \ 1], -1)$. You are orthogonalizing the columns $(1, -1, 0, 0)$ and $(0, 1, -1, 0)$ and $(0, 0, 1, -1)$ and $(0, 0, 0, 1)$ of A. Can you scale the orthogonal columns of Q to get nice integer components?

36 If A is m by n with rank n, $\mathbf{qr}(A)$ produces a *square* Q and zeros below R:

The factors from MATLAB are $(m \text{ by } m)(m \text{ by } n)$ $\qquad A = [Q_1 \quad Q_2] \begin{bmatrix} R \\ 0 \end{bmatrix}.$

The n columns of Q_1 are an orthonormal basis for which fundamental subspace? The $m-n$ columns of Q_2 are an orthonormal basis for which fundamental subspace?

37 We know that $P = QQ^{\mathrm{T}}$ is the projection onto the column space of $Q(m \text{ by } n)$. Now add another column $\boldsymbol{a}$ to produce $A = [Q \quad \boldsymbol{a}]$. Gram-Schmidt replaces $\boldsymbol{a}$ by what vector $\boldsymbol{q}$? Start with $\boldsymbol{a}$, subtract _____, divide by _____ to find $\boldsymbol{q}$.