5.4 Projection matrices

Review. To compute the orthogonal projection $\hat{\boldsymbol{b}}$ of $\boldsymbol{b}$ onto W, we have two options:

- **(using least squares)** Write $W = \operatorname{col}(A)$, where the columns of A are a basis of W. Then, $\hat{\boldsymbol{b}} = A\hat{\boldsymbol{x}}$ where $\hat{\boldsymbol{x}}$ is the least squares solution to $A\boldsymbol{x} = \boldsymbol{b}$ (i.e. $A^T A\hat{\boldsymbol{x}} = A^T\boldsymbol{b}$).
- **(using orthogonality)** If $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_m$ is an orthogonal basis of W, then

$$\hat{\boldsymbol{b}} = \left(\frac{\boldsymbol{b}\cdot\boldsymbol{v}_1}{\boldsymbol{v}_1\cdot\boldsymbol{v}_1}\right)\boldsymbol{v}_1 + \ldots + \left(\frac{\boldsymbol{b}\cdot\boldsymbol{v}_m}{\boldsymbol{v}_m\cdot\boldsymbol{v}_m}\right)\boldsymbol{v}_m.$$

In the least squares approach, assuming $A^T A$ is invertible (which, by Example 45, is automatically the case if the columns of A are independent), we have $\hat{\boldsymbol{x}} = (A^T A)^{-1} A^T \boldsymbol{b}$ and hence:

(projection matrix) The projection $\hat{\boldsymbol{b}}$ of $\boldsymbol{b}$ onto $\operatorname{col}(A)$ is

$$\hat{\boldsymbol{b}} = \underbrace{A(A^T A)^{-1} A^T}_{P}\boldsymbol{b}.$$

The matrix $P = A(A^T A)^{-1} A^T$ is the **projection matrix** for projecting onto $\operatorname{col}(A)$.

Example 66.

(a) Determine the projection matrix P for projecting onto $W = \operatorname{span}\left\{\begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}\right\}$

(b) Determine (once more!) the projection of $\begin{bmatrix} 3 \\ 7 \\ 4 \end{bmatrix}$ onto W using the projection matrix.

Solution.

(a) Choosing $A = \begin{bmatrix} 1 & 0 \\ -1 & 0 \\ 0 & 1 \end{bmatrix}$, the projection matrix P is $A(A^T A)^{-1} A^T = \begin{bmatrix} 1 & 0 \\ -1 & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix}^{-1}\begin{bmatrix} 1 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$ $= \begin{bmatrix} 1 & 0 \\ -1 & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} 1/2 & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} 1 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1/2 & -1/2 & 0 \\ -1/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{bmatrix}$.

(b) The projection of $\begin{bmatrix} 3 \\ 7 \\ 4 \end{bmatrix}$ onto W is $\begin{bmatrix} 1/2 & -1/2 & 0 \\ -1/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} 3 \\ 7 \\ 4 \end{bmatrix} = \begin{bmatrix} -2 \\ 2 \\ 4 \end{bmatrix}$.

This is, of course, exactly the answer we found in Example 64.

Comment. You can choose A in any way such that its columns are a basis for W. The final projection matrix will always be the same.

Example 67. (homework) If P is a projection matrix, then what is P^2?

For instance. For P as in the previous example, $P^2 = \begin{bmatrix} 1/2 & -1/2 & 0 \\ -1/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{bmatrix}^2 = \begin{bmatrix} 1/2 & -1/2 & 0 \\ -1/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{bmatrix} = P$.

Solution. Can you see why it is always true that $P^2 = P$?

[Recall that P projects a vector onto a space W (actually, $W = \operatorname{col}(P)$). Hence P^2 takes a vector $\boldsymbol{b}$, projects it onto W to get $\hat{\boldsymbol{b}}$, and then projects $\hat{\boldsymbol{b}}$ onto W again. But the projection of $\hat{\boldsymbol{b}}$ onto W is just $\hat{\boldsymbol{b}}$ (why?!), so that P^2 always has the exact same effect as P. Therefore, $P^2 = P$.]

Example 68. (homework)

(a) What is the matrix P for projecting onto $W = \operatorname{span}\left\{ \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix} \right\}$?

(b) Using the projection matrix, project $\begin{bmatrix} 2 \\ 3 \\ 3 \end{bmatrix}$ onto $W = \operatorname{span}\left\{ \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix} \right\}$.

Solution.

(a) Choosing $A = \begin{bmatrix} 1 & 1 \\ 1 & -1 \\ 1 & 1 \end{bmatrix}$, the projection matrix P is $A(A^TA)^{-1}A^T = \begin{bmatrix} 1 & 1 \\ 1 & -1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 3 & 1 \\ 1 & 3 \end{bmatrix}^{-1} \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \end{bmatrix}$

$= \begin{bmatrix} 1 & 1 \\ 1 & -1 \\ 1 & 1 \end{bmatrix} \frac{1}{8} \begin{bmatrix} 3 & -1 \\ -1 & 3 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \end{bmatrix} = \frac{1}{8} \begin{bmatrix} 1 & 1 \\ 1 & -1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 2 & 4 & 2 \\ 2 & -4 & 2 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix}$.

(b) The projection is $\frac{1}{2} \begin{bmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 3 \\ 3 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 5 \\ 6 \\ 5 \end{bmatrix}$.

Check. The error $\begin{bmatrix} 2 \\ 3 \\ 3 \end{bmatrix} - \frac{1}{2} \begin{bmatrix} 5 \\ 6 \\ 5 \end{bmatrix} = \begin{bmatrix} -1/2 \\ 0 \\ 1/2 \end{bmatrix}$ is indeed orthogonal to W.

5.5 Gram–Schmidt

Example 69. Find an orthogonal basis for $W = \operatorname{span}\left\{ \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix} \right\}$.

Solution. We already have the basis $\boldsymbol{w}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$, $\boldsymbol{w}_2 = \begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix}$ for W. However, that basis is not orthogonal.

We can construct an orthogonal basis $\boldsymbol{q}_1, \boldsymbol{q}_2$ for W as follows:

- $\boldsymbol{q}_1 = \boldsymbol{w}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$

  Since this is our first basis vector, we don't yet have other basis vectors it needs to be orthogonal to.

- $\boldsymbol{q}_2 = \boldsymbol{w}_2 - \begin{pmatrix} \text{projection of} \\ \boldsymbol{w}_2 \text{ onto } \boldsymbol{q}_1 \end{pmatrix} = \begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix} - \frac{1}{3} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 2/3 \\ -4/3 \\ 2/3 \end{bmatrix}$

  Make sure our way to construct $\boldsymbol{q}_2$ makes sense to you!
  $\boldsymbol{q}_2$ is the error of the projection of $\boldsymbol{w}_2$ onto $\boldsymbol{q}_1$. This guarantees that it is orthogonal to $\boldsymbol{q}_1$.
  On the other hand, since $\boldsymbol{q}_2$ is a combination of $\boldsymbol{w}_2$ and $\boldsymbol{q}_1$, we know that $\boldsymbol{q}_2$ actually is in W.

We have thus found the orthogonal basis $\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 2/3 \\ -4/3 \\ 2/3 \end{bmatrix}$ for W.

Important comment. Normalizing these, we get $\frac{1}{\sqrt{3}} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, \frac{1}{\sqrt{6}} \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}$, which is an orthonormal basis for W.

Comment. There are, of course, many orthogonal bases $\boldsymbol{q}_1, \boldsymbol{q}_2$ for W. Up to the length of the vectors, ours is the unique one with the property that $\operatorname{span}\{\boldsymbol{q}_1\} = \operatorname{span}\{\boldsymbol{w}_1\}$ and $\operatorname{span}\{\boldsymbol{q}_1, \boldsymbol{q}_2\} = \operatorname{span}\{\boldsymbol{w}_1, \boldsymbol{w}_2\}$.

Example 70. Extend the previous basis to an orthogonal basis of $\operatorname{span}\left\{\begin{bmatrix}1\\1\\1\end{bmatrix},\begin{bmatrix}1\\-1\\1\end{bmatrix},\begin{bmatrix}1\\0\\2\end{bmatrix}\right\}$.

[Of course, this span is all of $\mathbb{R}^3$.]

Solution. Let us repeat the previous step so the entire procedure becomes more transparent.

We begin with the (not orthogonal) basis $\boldsymbol{w}_1=\begin{bmatrix}1\\1\\1\end{bmatrix}$, $\boldsymbol{w}_2=\begin{bmatrix}1\\-1\\1\end{bmatrix}$, $\boldsymbol{w}_3=\begin{bmatrix}1\\0\\2\end{bmatrix}$.

We then construct an orthogonal basis $\boldsymbol{q}_1,\boldsymbol{q}_2,\boldsymbol{q}_3$ as follows:

- $\boldsymbol{q}_1=\boldsymbol{w}_1=\begin{bmatrix}1\\1\\1\end{bmatrix}$
- $\boldsymbol{q}_2=\boldsymbol{w}_2-\left(\begin{array}{c}\text{projection of}\\ \boldsymbol{w}_2 \text{ onto } \boldsymbol{q}_1\end{array}\right)=\begin{bmatrix}1\\-1\\1\end{bmatrix}-\frac{1}{3}\begin{bmatrix}1\\1\\1\end{bmatrix}=\begin{bmatrix}2/3\\-4/3\\2/3\end{bmatrix}$
- $\boldsymbol{q}_3=\boldsymbol{w}_3-\left(\begin{array}{c}\text{projection of } \boldsymbol{w}_3\\ \text{onto } \operatorname{span}\{\boldsymbol{q}_1,\boldsymbol{q}_2\}\end{array}\right)=\boldsymbol{w}_3-\left(\begin{array}{c}\text{projection of}\\ \boldsymbol{w}_3 \text{ onto } \boldsymbol{q}_1\end{array}\right)-\left(\begin{array}{c}\text{projection of}\\ \boldsymbol{w}_3 \text{ onto } \boldsymbol{q}_2\end{array}\right)$
  $=\begin{bmatrix}1\\0\\2\end{bmatrix}-\begin{bmatrix}1\\1\\1\end{bmatrix}-\frac{1}{4}\begin{bmatrix}2\\-4\\2\end{bmatrix}=\frac{1}{2}\begin{bmatrix}-1\\0\\1\end{bmatrix}$

  Make sure you see why $\boldsymbol{q}_3$ is orthogonal to both $\boldsymbol{q}_1$ and $\boldsymbol{q}_2$!

  Also note that breaking up the projection onto $\operatorname{span}\{\boldsymbol{q}_1,\boldsymbol{q}_2\}$ into the projections onto $\boldsymbol{q}_1$ and $\boldsymbol{q}_2$ is only possible because $\boldsymbol{q}_1$ and $\boldsymbol{q}_2$ are orthogonal.

Indeed, $\begin{bmatrix}1\\1\\1\end{bmatrix},\frac{2}{3}\begin{bmatrix}1\\-2\\1\end{bmatrix},\frac{1}{2}\begin{bmatrix}-1\\0\\1\end{bmatrix}$ is an orthogonal basis of $\mathbb{R}^3$.

If we prefer, we can normalize to obtain an orthonormal basis: $\frac{1}{\sqrt{3}}\begin{bmatrix}1\\1\\1\end{bmatrix},\frac{1}{\sqrt{6}}\begin{bmatrix}1\\-2\\1\end{bmatrix},\frac{1}{\sqrt{2}}\begin{bmatrix}-1\\0\\1\end{bmatrix}$.

(Gram–Schmidt orthogonalization)

Given a basis $\boldsymbol{w}_1,\boldsymbol{w}_2,\ldots$ for W, produce an orthogonal basis $\boldsymbol{q}_1,\boldsymbol{q}_2,\ldots$ for W.

- $\boldsymbol{q}_1=\boldsymbol{w}_1$
- $\boldsymbol{q}_2=\boldsymbol{w}_2-\left(\begin{array}{c}\text{projection of}\\ \boldsymbol{w}_2 \text{ onto } \boldsymbol{q}_1\end{array}\right)$
- $\boldsymbol{q}_3=\boldsymbol{w}_3-\left(\begin{array}{c}\text{projection of}\\ \boldsymbol{w}_3 \text{ onto } \boldsymbol{q}_1\end{array}\right)-\left(\begin{array}{c}\text{projection of}\\ \boldsymbol{w}_3 \text{ onto } \boldsymbol{q}_2\end{array}\right)$
- $\boldsymbol{q}_4=\ldots$

Important comment. When working numerically it actually saves time to compute an orthonormal basis $\boldsymbol{q}_1,\boldsymbol{q}_2,\ldots$ by the same approach but always normalizing each $\boldsymbol{q}_i$ along the way. The reason this saves time is that now the projections onto $\boldsymbol{q}_i$ only require a single dot product (instead of two). This is called **Gram–Schmidt orthonormalization**.

Note. When normalizing, the orthonormal basis $\boldsymbol{q}_1,\boldsymbol{q}_2,\ldots$ is the unique one with the property that $\operatorname{span}\{\boldsymbol{q}_1,\boldsymbol{q}_2,\ldots,\boldsymbol{q}_k\}=\operatorname{span}\{\boldsymbol{w}_1,\boldsymbol{w}_2,\ldots,\boldsymbol{w}_k\}$ for all $k=1,2,\ldots$.