Example 61. Using Gram–Schmidt, find an orthogonal basis for $W = \text{span}\left\{ \begin{bmatrix} 0 \\ 3 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 2 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \right\}$.

Solution. We begin with the (not orthogonal) basis $\boldsymbol{w}_1 = \begin{bmatrix} 0 \\ 3 \\ 0 \\ 0 \end{bmatrix}$, $\boldsymbol{w}_2 = \begin{bmatrix} 2 \\ 1 \\ 0 \\ 0 \end{bmatrix}$, $\boldsymbol{w}_3 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$.

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

- $\boldsymbol{q}_1 = \boldsymbol{w}_1 = \begin{bmatrix} 0 \\ 3 \\ 0 \\ 0 \end{bmatrix}$
- $\boldsymbol{q}_2 = \boldsymbol{w}_2 - \begin{pmatrix} \text{projection of} \\ \boldsymbol{w}_2 \text{ onto } \boldsymbol{q}_1 \end{pmatrix} = \begin{bmatrix} 2 \\ 1 \\ 0 \\ 0 \end{bmatrix} - \frac{3}{9} \begin{bmatrix} 0 \\ 3 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 2 \\ 0 \\ 0 \\ 0 \end{bmatrix}$
- $\boldsymbol{q}_3 = \boldsymbol{w}_3 - \begin{pmatrix} \text{projection of } \boldsymbol{w}_3 \\ \text{onto span}\{\boldsymbol{q}_1, \boldsymbol{q}_2\} \end{pmatrix} = \boldsymbol{w}_3 - \begin{pmatrix} \text{projection of} \\ \boldsymbol{w}_3 \text{ onto } \boldsymbol{q}_1 \end{pmatrix} - \begin{pmatrix} \text{projection of} \\ \boldsymbol{w}_3 \text{ onto } \boldsymbol{q}_2 \end{pmatrix}$
  $= \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} - \frac{3}{9} \begin{bmatrix} 0 \\ 3 \\ 0 \\ 0 \end{bmatrix} - \frac{2}{4} \begin{bmatrix} 2 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$
  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 $\text{span}\{\boldsymbol{q}_1, \boldsymbol{q}_2\}$ 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, $\begin{bmatrix} 0 \\ 3 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 2 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$ is an orthogonal basis of $\mathbb{R}^3$.

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

It is common and beneficial (slightly less work) to normalize during the Gram–Schmidt process. We do this in Example 62 below.

The following is just the Gram–Schmidt orthogonalization except that we immediately normalize each vector $\boldsymbol{q}_i$.

(Gram–Schmidt orthonormalization)

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

- $\boldsymbol{q}_1 = \frac{\boldsymbol{b}_1}{\|\boldsymbol{b}_1\|}$ with $\boldsymbol{b}_1 = \boldsymbol{w}_1$
- $\boldsymbol{q}_2 = \frac{\boldsymbol{b}_2}{\|\boldsymbol{b}_2\|}$ with $\boldsymbol{b}_2 = \boldsymbol{w}_2 - (\boldsymbol{w}_2 \cdot \boldsymbol{q}_1)\boldsymbol{q}_1$
- $\boldsymbol{q}_3 = \frac{\boldsymbol{b}_3}{\|\boldsymbol{b}_3\|}$ with $\boldsymbol{b}_3 = \boldsymbol{w}_3 - (\boldsymbol{w}_3 \cdot \boldsymbol{q}_1)\boldsymbol{q}_1 - (\boldsymbol{w}_3 \cdot \boldsymbol{q}_2)\boldsymbol{q}_2$
- $\boldsymbol{q}_4 = \ldots$

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Example 62. Find an orthonormal basis for $W = \operatorname{span}\left\{ \begin{bmatrix} 0 \\ 3 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 2 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \right\}$.

Solution. Let $\boldsymbol{w}_1, \boldsymbol{w}_2, \boldsymbol{w}_3$ be the vectors spaning W. We then construct an orthonormal basis $\boldsymbol{q}_1, \boldsymbol{q}_2, \boldsymbol{q}_3$ using Gram–Schmidt orthonormalization as follows:

- $\boldsymbol{b}_1 = \begin{bmatrix} 0 \\ 3 \\ 0 \\ 0 \end{bmatrix}$, so that $\boldsymbol{q}_1 = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$.
- $\boldsymbol{b}_2 = \begin{bmatrix} 2 \\ 1 \\ 0 \\ 0 \end{bmatrix} - \left(\begin{bmatrix} 2 \\ 1 \\ 0 \\ 0 \end{bmatrix} \cdot \boldsymbol{q}_1 \right) \boldsymbol{q}_1 = \begin{bmatrix} 2 \\ 0 \\ 0 \\ 0 \end{bmatrix}$, so that $\boldsymbol{q}_2 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$.
- $\boldsymbol{b}_3 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} - \left(\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \cdot \boldsymbol{q}_1 \right) \boldsymbol{q}_1 - \left(\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \cdot \boldsymbol{q}_2 \right) \boldsymbol{q}_2 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$, so that $\boldsymbol{q}_3 = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$.

We have found the orthonormal basis: $\begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$ (which, of course, matches the previous example).

A matrix Q has orthonormal columns $\iff$ $Q^T Q = I$

Why? Let $\boldsymbol{q}_1, \boldsymbol{q}_2, \ldots$ be the columns of Q. By the way matrix multiplication works, the entries of $Q^T Q$ are dot products of these columns:

$$\begin{bmatrix} — & \boldsymbol{q}_1^T & — \\ — & \boldsymbol{q}_2^T & — \\ & \vdots & \end{bmatrix} \begin{bmatrix} | & | & \\ \boldsymbol{q}_1 & \boldsymbol{q}_2 & \cdots \\ | & | & \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \ddots \end{bmatrix}$$

Hence, $Q^T Q = I$ if and only if the dot products $\boldsymbol{q}_i^T \boldsymbol{q}_j = 0$ (that is, the columns are orthogonal), for $i \neq j$, and $\boldsymbol{q}_i^T \boldsymbol{q}_i = 1$ (that is, the columns are normalized).

Example 63. $Q = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1/\sqrt{2} \\ 0 & 0 & 1/\sqrt{2} \end{bmatrix}$ obtained from the previous example satisfies $Q^T Q = I$.

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The QR decomposition

Just like the LU decomposition encodes the steps of Gaussian elimination, the QR decomposition encodes the steps of Gram–Schmidt.

(QR decomposition) Every $m \times n$ matrix A of rank n can be decomposed as $A = QR$, where

- Q has orthonormal columns, $(m \times n)$
- R is upper triangular and invertible. $(n \times n)$

How to find Q and R?

- Gram–Schmidt orthonormalization on (columns of) A, to get (columns of) Q
- $R = Q^T A$
  Why? If $A = QR$, then $Q^T A = Q^T Q R$ which simplifies to $R = Q^T A$ (since $Q^T Q = I$).

The decomposition $A = QR$ is unique if we require the diagonal entries of R to be positive (and this is exactly what happens when applying Gram–Schmidt).

Practical comment. Actually, no extra work is needed for computing R. All of its entries have been computed during Gram–Schmidt.

Variations. We can also arrange things so that Q is an $m \times m$ orthogonal matrix and R a $m \times n$ upper triangular matrix. This is a tiny bit more work (and not required for many applications): we need to complement "our" Q with additional orthonormal columns and add corresponding zero rows to R. For square matrices this makes no difference.

Example 64. Determine the QR decomposition of $A = \begin{bmatrix} 0 & 2 & 1 \\ 3 & 1 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix}$.

Solution. The first step is Gram–Schmidt orthonormalization on the columns of A. We then use the resulting orthonormal vectors as the columns of Q.

We already did Gram–Schmidt in Example 62: from that work, we have $Q = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1/\sqrt{2} \\ 0 & 0 & 1/\sqrt{2} \end{bmatrix}$.

Hence, $R = Q^T A = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix} \begin{bmatrix} 0 & 2 & 1 \\ 3 & 1 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 3 & 1 & 1 \\ 0 & 2 & 1 \\ 0 & 0 & \sqrt{2} \end{bmatrix}$.

Comment. As commented earlier, the entries of R have actually all been computed during Gram–Schmidt, so that, if we pay attention, we could immediately write down R (no extra work required). Looking back at Example 62, can you see this?

Check. Indeed, $QR = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1/\sqrt{2} \\ 0 & 0 & 1/\sqrt{2} \end{bmatrix} \begin{bmatrix} 3 & 1 & 1 \\ 0 & 2 & 1 \\ 0 & 0 & \sqrt{2} \end{bmatrix} = \begin{bmatrix} 0 & 2 & 1 \\ 3 & 1 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix}$ equals A.

Example 65. (extra) Find the QR decomposition of $A = \begin{bmatrix} 1 & 1 & 2 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$.

Solution. (final answer only) $A = QR$ with $Q = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{bmatrix}$ and $R = \begin{bmatrix} \sqrt{2} & \frac{1}{\sqrt{2}} & \sqrt{2} \\ 0 & \frac{1}{\sqrt{2}} & \sqrt{2} \\ 0 & 0 & 1 \end{bmatrix}$.