Gram-schmidt와 QR Decomposition

Gram-Schmidt Orthogonalization

- **Example 1**: Let $W = \mathrm{Span}\{\mathbf{x}_1, \mathbf{x}_2\}$, where $\mathbf{x}_1 = \begin{bmatrix} 3 \\ 6 \\ 0 \end{bmatrix}$ and $\mathbf{x}_2 = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}$. Construct an orthogonal basis $\{\mathbf{v}_1, \mathbf{v}_2\}$ for W.

- **Solution:** Let $\mathbf{v}_1 = \mathbf{x}_1$. Next, Let $\mathbf{v}_2$ the component of $\mathbf{x}_2$ orthogonal to $\mathbf{x}_1$, i.e.,

$$\mathbf{v}_2 = \mathbf{x}_2 - \frac{\mathbf{x}_2 \cdot \mathbf{x}_1}{\mathbf{x}_1 \cdot \mathbf{x}_1}\mathbf{x}_1 = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix} - \frac{15}{45}\begin{bmatrix} 3 \\ 6 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix}.$$

- The set $\{\mathbf{v}_1, \mathbf{v}_2\}$ is an orthogonal basis for W.

Gram-Schmidt Orthogonalization

- **Example 2**: Let $\mathbf{x}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$, $\mathbf{x}_2 = \begin{bmatrix} 0 \\ 1 \\ 1 \\ 1 \end{bmatrix}$, and $\mathbf{x}_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$. Then $\{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3\}$ is clearly linearly independent and thus a basis for a subspace W of $\mathbb{R}^4$. Construct an orthogonal basis for W.

Gram-Schmidt Orthogonalization

- **Solution:**
- **Step 1.** Let $\mathbf{v}_1 = \mathbf{x}_1$ and $W_1 = \mathrm{Span}\{\mathbf{x}_1\} = \mathrm{Span}\{\mathbf{v}_1\}$.
- **Step 2.** Let $\mathbf{v}_2$ be the vector produced by subtracting from $\mathbf{x}_2$ its projection onto the subspace W_1. That is, let

$$\mathbf{v}_2 = \mathbf{x}_2 - \mathrm{proj}_{W_1}\mathbf{x}_2 = \mathbf{x}_2 - \frac{\mathbf{x}_2 \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1}\mathbf{v}_1 = \begin{bmatrix} -3/4 \\ 1/4 \\ 1/4 \\ 1/4 \end{bmatrix}$$

- $\mathbf{v}_2$ is the component of $\mathbf{x}_2$ orthogonal to $\mathbf{x}_1$, and $\{\mathbf{v}_1, \mathbf{v}_2\}$ is an orthogonal basis for the subspace W_2 spanned by $\mathbf{x}_1$ and $\mathbf{x}_2$.

Gram-Schmidt Orthogonalization

- **Step 2' (optional).** If appropriate, scale $\mathbf{v}_2$ to simplify later computations, e.g.,

$$\mathbf{v}_2 = \begin{bmatrix} -3/4 \\ 1/4 \\ 1/4 \\ 1/4 \end{bmatrix} \longrightarrow \mathbf{v}_2' = \begin{bmatrix} -3 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

Gram-Schmidt Orthogonalization

- **Step 3.** Let $\mathbf{v}_3$ be the vector produced by subtracting from $\mathbf{x}_3$ its projection onto the subspace W_2. Use the orthogonal basis $\{\mathbf{v}_1, \mathbf{v}_2'\}$ to compute this projection onto W_2:

$$\text{proj}_{W_2}\mathbf{x}_3 = \frac{\mathbf{x}_3 \cdot \mathbf{v}_1}{\mathbf{v}_3 \cdot \mathbf{v}_1}\mathbf{v}_1 + \frac{\mathbf{x}_3 \cdot \mathbf{v}_2'}{\mathbf{v}_3 \cdot \mathbf{v}_2'}\mathbf{v}_2' = \begin{bmatrix} 0 \\ 2/3 \\ 2/3 \\ 2/3 \end{bmatrix}$$

- Then $\mathbf{v}_3$ is the component of $\mathbf{x}_3$ orthogonal to W_2, namely,

$$\mathbf{v}_3 = \mathbf{x}_3 - \text{proj}_{W_2}\mathbf{x}_3 = \begin{bmatrix} 0 \\ -2/3 \\ 1/3 \\ 1/3 \end{bmatrix}$$

Gram-Schmidt Orthogonalization

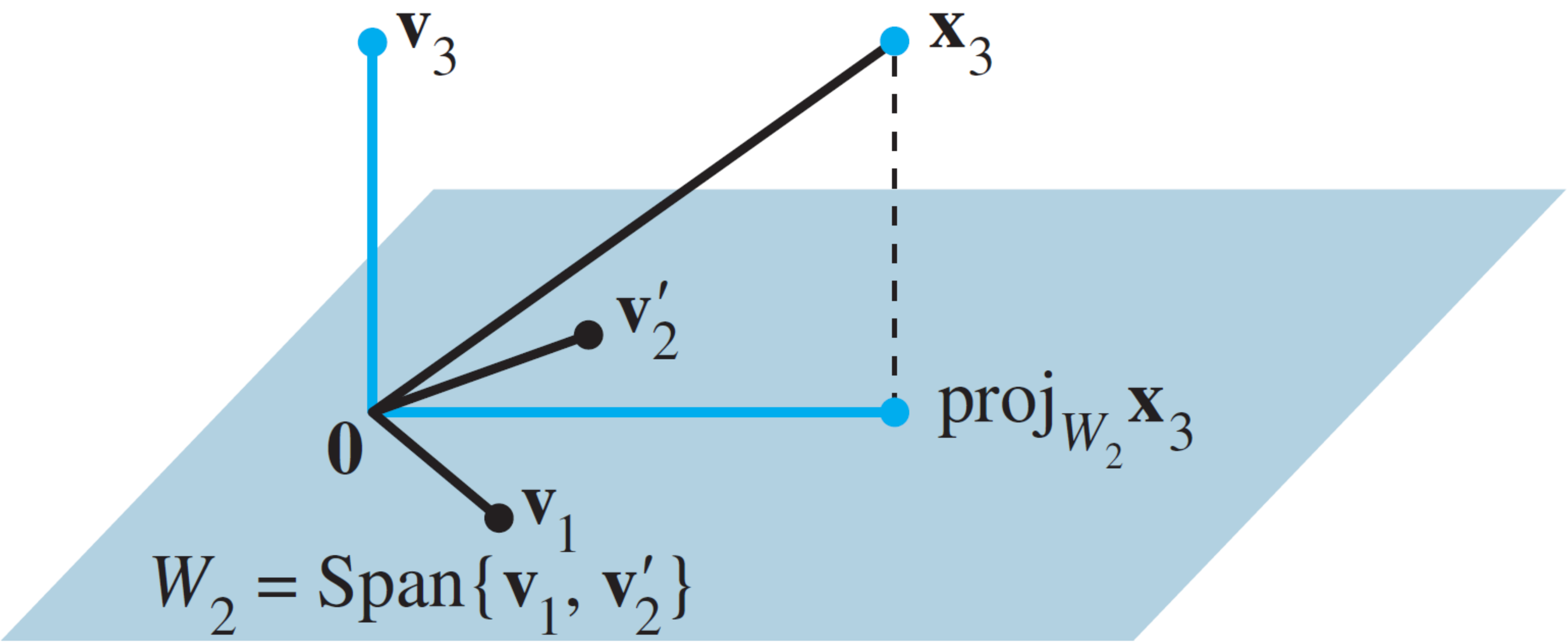

FIGURE 2 The construction of $\mathbf{v}_3$ from $\mathbf{x}_3$ and W_2.

Figure from Lay Ch6.4

QR Factorization

- If A is an $m \times n$ matrix with linearly independent columns, then A can be factored as $A = QR$, where Q is an $m \times n$ matrix whose columns form an orthonormal basis for $\mathrm{Col}\, A$ and R is an $n \times n$ upper triangular invertible matrix with positive entries on its diagonal.

Computing QR Factorization

- **Step 1 (Construction of Q):** The columns of A form a basis for $\mathrm{Col}\,A$ since they are linearly independent. Let these columns be $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$. Then, we can construct the orthonormal basis $\{\mathbf{u}_1, \ldots, \mathbf{u}_n\}$ for $\mathrm{Col}\,A$ by the Gram-Schmidt process described by Theorem 11. Using this basis, we can construct Q as

$$Q = [\mathbf{u}_1 \quad \mathbf{u}_2 \quad \cdots \quad \mathbf{u}_n]$$

Computing QR Factorization

- **Step 2 (Construction of R):** From (1) in Theorem 11, for $k = 1, \dots, n$, $\mathbf{x}_k$ is in $\mathrm{Span}\{\mathbf{x}_1, \dots, \mathbf{x}_k\} = \mathrm{Span}\{\mathbf{u}_1, \dots, \mathbf{u}_k\}$. Therefore, there exist constants $r_{1k}, \dots, r_{kk}$ such that

$$\mathbf{x}_k = r_{1k}\mathbf{u}_1 + \cdots + r_{kk}\mathbf{u}_k + 0 \cdot \mathbf{u}_{k+1} + \cdots + 0 \cdot \mathbf{u}_n$$

- We can always make $r_{kk} \geq 0$ because if $r_{kk} < 0$, then we can multiply both r_{kk} and $\mathbf{u}_k$ by -1. Using this linear combination representation, we can construct $\mathbf{r}_k$, the k-th column of R, as

$$\mathbf{r}_k = \begin{bmatrix} r_{1k} \\ \vdots \\ r_{kk} \\ 0 \\ \vdots \\ 0 \end{bmatrix}.$$

Computing QR Factorization

- That is, $\mathbf{x}_k = Q\mathbf{r}_k$ for $k = 1, \dots, n$. Let $R = [\mathbf{r}_1 \quad \cdots \quad \mathbf{r}_n]$. Then,
$$A = [\mathbf{x}_1 \quad \cdots \quad \mathbf{x}_n] = [Q\mathbf{r}_1 \quad \cdots \quad Q\mathbf{r}_n] = QR$$

- The fact that R is invertible follows easily from the fact that the columns of A are linearly independent (Exercise 19). Since R is clearly upper triangular (from the previous slide) and invertible, the diagonal entries r_{kk}'s should be nonzero. By combining this with the fact that $r_{kk} \geq 0$, r_{kk}'s must be positive.

Example: QR Factorization

- **Example 4:** Find a QR factorization of $A = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$.
- **Solution:** Let $A = [\mathbf{x}_1 \quad \mathbf{x}_2 \quad \mathbf{x}_3]$. We first obtain $\mathbf{v}_1 = \mathbf{x}_1$ and its normalized vector is $\mathbf{u}_1 = \frac{1}{\|\mathbf{v}_1\|}\mathbf{v}_1 = \frac{1}{\sqrt{1^2+1^2+1^2+1^2}}\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1/2 \\ 1/2 \\ 1/2 \\ 1/2 \end{bmatrix}$.
- Thus, $\mathbf{x}_1 = 2\mathbf{u}_1$, which gives us $\mathbf{r}_{11} = 2$, i.e., $\mathbf{r}_1 = \begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix}$.

Example: QR Factorization

- Next, we obtain $\mathbf{v}_2$ as $\mathbf{v}_2 = \mathbf{x}_2 - \mathrm{proj}_{W_1}\mathbf{x}_2 = \mathbf{x}_2 - (\mathbf{x}_2 \cdot \mathbf{u}_1)\mathbf{u}_1 = \begin{bmatrix} 0 \\ 1 \\ 1 \\ 1 \end{bmatrix} - \frac{3}{2}\begin{bmatrix} 1/2 \\ 1/2 \\ 1/2 \\ 1/2 \end{bmatrix} = \begin{bmatrix} -3/4 \\ 1/4 \\ 1/4 \\ 1/4 \end{bmatrix}$ and its normalized vector $\mathbf{u}_2$ as

$$\mathbf{u}_2 = \frac{1}{\|\mathbf{v}_2\|}\mathbf{v}_2 = \frac{1}{\sqrt{3}/2}\begin{bmatrix} -3/4 \\ 1/4 \\ 1/4 \\ 1/4 \end{bmatrix} = \begin{bmatrix} -\sqrt{3}/2 \\ \sqrt{3}/6 \\ \sqrt{3}/6 \\ \sqrt{3}/6 \end{bmatrix}.$$

- Thus, $\mathbf{x}_2 = \frac{3}{2}\mathbf{u}_1 + \frac{\sqrt{3}}{2}\mathbf{u}_2$, i.e., $\mathbf{r}_2 = \begin{bmatrix} 3/2 \\ \sqrt{3}/2 \\ 0 \end{bmatrix}$.

Example: QR Factorization

- Next, we obtain $\mathbf{v}_3$ as $\mathbf{v}_3 = \mathbf{x}_3 - \mathrm{proj}_{W_2}\mathbf{x}_3 = \mathbf{x}_3 - (\mathbf{x}_3 \cdot \mathbf{u}_1)\mathbf{u}_1 - (\mathbf{x}_3 \cdot \mathbf{u}_2)\mathbf{u}_2 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix} - 1 \begin{bmatrix} 1/2 \\ 1/2 \\ 1/2 \\ 1/2 \end{bmatrix} - \frac{1}{\sqrt{3}} \begin{bmatrix} -\sqrt{3}/2 \\ \sqrt{3}/6 \\ \sqrt{3}/6 \\ \sqrt{3}/6 \end{bmatrix} = \begin{bmatrix} 0 \\ -2/3 \\ 1/3 \\ 1/3 \end{bmatrix}$ and its normalized vector $\mathbf{u}_3$ as $\mathbf{u}_3 = \frac{1}{\|\mathbf{v}_3\|}\mathbf{v}_3 = \frac{1}{2/\sqrt{6}} \begin{bmatrix} 0 \\ -2/3 \\ 1/3 \\ 1/3 \end{bmatrix} = \begin{bmatrix} 0 \\ -2/\sqrt{6} \\ 1/\sqrt{6} \\ 1/\sqrt{6} \end{bmatrix}$.
- Thus, $\mathbf{x}_3 = 1\mathbf{u}_1 + \frac{1}{\sqrt{3}}\mathbf{u}_2 + \frac{2}{\sqrt{6}}\mathbf{u}_3$, i.e., $\mathbf{r}_3 = \begin{bmatrix} 1 \\ 1/\sqrt{3} \\ 2/\sqrt{6} \end{bmatrix}$.

Example: QR Factorization

- In conclusion, $Q = [\mathbf{u}_1 \quad \mathbf{u}_2 \quad \mathbf{u}_3] = \begin{bmatrix} 1/2 & -\sqrt{3}/2 & 0 \\ 1/2 & \sqrt{3}/6 & -2/\sqrt{6} \\ 1/2 & \sqrt{3}/6 & 1/\sqrt{6} \\ 1/2 & \sqrt{3}/6 & 1/\sqrt{6} \end{bmatrix}$

  and $R = [\mathbf{r}_1 \quad \mathbf{r}_2 \quad \mathbf{r}_3] = \begin{bmatrix} 2 & 3/2 & 1 \\ 0 & \sqrt{3}/2 & 1/\sqrt{3} \\ 0 & 0 & 2/\sqrt{6} \end{bmatrix}$.