Linear Algebra
[KOMS120301] - 2023/2024

15.2 - Gram-Schmidt & QR-Decomposition

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Learning objectives

After this lecture, you should be able to:

1. explain the concepts of orthogonal set and orthonormal set;
2. explain the procedure of Gram-Schmidt;
3. perform the procedure of Gram-Schmidt to get an orthonormal basis;
4. explain the procedure of QR-decomposition;
5. find a QR-decomposition of a matrix.

Part 1: Orthogonal and orthonormal sets

Orthogonal and orthonormal sets

Let S be a set of two or more vectors in a real inner product space. Then:

- S is said to be orthogonal if all pairs of distinct vectors in the set are orthogonal.
- S is said to be orthonormal if S is orthogonal and $\forall v \in S$, $\|v\| = 1$.

Why do we need an orthogonal set or an orthonormal set?

Reference: `https://www.youtube.com/watch?v=SWbis2zWIvo`

Task: Find an example that shows the importance of an orthogonal or an orthonormal set in Linear Algebra.

Example 1: Orthogonal sets

Given vectors in $\mathbb{R}^3$:

$$\mathbf{v}_1 = (0, 1, 0), \quad \mathbf{v}_2 = (1, 0, 1), \quad \mathbf{v}_3 = (1, 0, -1)$$

with Euclidean inner product. Is the set $S = \{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3\}$ orthogonal?

Example 1: Orthogonal sets

Given vectors in $\mathbb{R}^3$:

$$\mathbf{v}_1 = (0, 1, 0), \quad \mathbf{v}_2 = (1, 0, 1), \quad \mathbf{v}_3 = (1, 0, -1)$$

with Euclidean inner product. Is the set $S = \{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3\}$ orthogonal?

Solution:

Show that $\langle \mathbf{v}_1, \mathbf{v}_2 \rangle = 0$, $\langle \mathbf{v}_1, \mathbf{v}_3 \rangle = 0$, and $\langle \mathbf{v}_2, \mathbf{v}_3 \rangle = 0$.

Example 2: Constructing an orthonormal set from an orthogonal set

From the previous example, we see that $S = \{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3\}$ is an orthogonal set. How to construct an orthonormal set out of it?

- The Euclidean norms of the vectors:

$$\|\mathbf{v}_1\| = 1,\ \|\mathbf{v}_2\| = \sqrt{2},\ \|\mathbf{v}_3\| = \sqrt{2}$$

- Normalizing $\mathbf{v}_1$, $\mathbf{v}_2$, and $\mathbf{v}_3$ yields:

$$\mathbf{u}_1 = \frac{\mathbf{v}_1}{\|\mathbf{v}_1\|}, \quad \mathbf{u}_2 = \frac{\mathbf{v}_2}{\|\mathbf{v}_2\|} = \left(\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}\right),$$

$$\mathbf{u}_3 = \frac{\mathbf{v}_3}{\|\mathbf{v}_3\|} = \left(\frac{1}{\sqrt{2}}, 0, -\frac{1}{\sqrt{2}}\right)$$

- Verify that

$$\langle \mathbf{u}_1, \mathbf{u}_2 \rangle = \langle \mathbf{u}_1, \mathbf{u}_3 \rangle = \langle \mathbf{u}_2, \mathbf{u}_3 \rangle = 0, \quad \text{and}$$

$$\|\mathbf{v}_1\| = 1,\ \|\mathbf{v}_2\| = 1,\ \|\mathbf{v}_3\| = 1$$

Hence, $\{\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3\}$ is an orthonormal set.

Exercises

Part 2: The Gram-Schmidt Process

Importance of orthogonal basis & orthonormal basis

Theorem (Orthogonal basis & orthonormal basis)

1. *If* $S = \{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n\}$ *is an orthogonal basis for an inner product space* V*, and if* u *is any vector in* V*, then:*

$$\mathbf{u} = \frac{\langle \mathbf{u}, \mathbf{v}_1 \rangle}{\|\mathbf{v}_1\|^2}\mathbf{v}_1 + \frac{\langle \mathbf{u}, \mathbf{v}_2 \rangle}{\|\mathbf{v}_2\|^2}\mathbf{v}_2 + \cdots + \frac{\langle \mathbf{u}, \mathbf{v}_n \rangle}{\|\mathbf{v}_n\|^2}\mathbf{v}_n$$

2. *If* $S = \{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n\}$ *is an orthonormal basis for an inner product space* V*, and if* u *is any vector in* V*, then:*

$$\mathbf{u} = \langle \mathbf{u}, \mathbf{v}_1 \rangle \mathbf{v}_1 + \langle \mathbf{u}, \mathbf{v}_2 \rangle \mathbf{v}_2 + \cdots + \langle \mathbf{u}, \mathbf{v}_n \rangle \mathbf{v}_n$$

Does an *orthonormal basis* always exist?

Theorem

Every nonzero finite-dimensional inner product space has an **orthonormal basis***.*

The Gram-Schmidt Process (1)

The Gram-Schmidt process is the step-by-step construction of an orthogonal (or orthonormal) basis.

The Gram–Schmidt Process

To convert a basis $\{\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_r\}$ into an orthogonal basis $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_r\}$, perform the following computations:

Step 1. $\mathbf{v}_1 = \mathbf{u}_1$

Step 2. $\mathbf{v}_2 = \mathbf{u}_2 - \dfrac{\langle \mathbf{u}_2, \mathbf{v}_1 \rangle}{\|\mathbf{v}_1\|^2}\mathbf{v}_1$

Step 3. $\mathbf{v}_3 = \mathbf{u}_3 - \dfrac{\langle \mathbf{u}_3, \mathbf{v}_1 \rangle}{\|\mathbf{v}_1\|^2}\mathbf{v}_1 - \dfrac{\langle \mathbf{u}_3, \mathbf{v}_2 \rangle}{\|\mathbf{v}_2\|^2}\mathbf{v}_2$

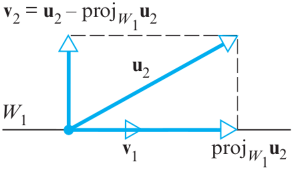
Step 4. $\mathbf{v}_4 = \mathbf{u}_4 - \dfrac{\langle \mathbf{u}_4, \mathbf{v}_1 \rangle}{\|\mathbf{v}_1\|^2}\mathbf{v}_1 - \dfrac{\langle \mathbf{u}_4, \mathbf{v}_2 \rangle}{\|\mathbf{v}_2\|^2}\mathbf{v}_2 - \dfrac{\langle \mathbf{u}_4, \mathbf{v}_3 \rangle}{\|\mathbf{v}_3\|^2}\mathbf{v}_3$

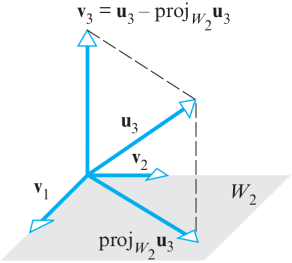
$\vdots$

(continue for r steps)

Optional Step. To convert the orthogonal basis into an orthonormal basis $\{\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_r\}$, normalize the orthogonal basis vectors.

The Gram-Schmidt Process (2)





Example 1: Gram-Schmidt process

Given vectors in $\mathbb{R}^3$:

$$\mathbf{u}_1 = (1,1,1),\ \mathbf{u}_2 = (0,1,1),\ \mathbf{u}_3 = (0,0,1)$$

1. Transfom the basis vectors into an orthogonal basis $\{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3\}$.
2. Normalize the orthogonal basis to obtain an orthonormal basis $\{\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3\}$.

Example 1 solution: Gram-Schmidt process

$$\mathbf{u}_1 = (1,1,1),\ \mathbf{u}_2 = (0,1,1),\ \mathbf{u}_3 = (0,0,1)$$

Step 1. $\mathbf{v}_1 = \mathbf{u}_1 = (1,1,1)$

Step 2. $\mathbf{v}_2 = \mathbf{u}_2 = \text{proj}_{W_1}\mathbf{u}_2 = \mathbf{u}_2 - \dfrac{\langle \mathbf{u}_2, \mathbf{v}_1 \rangle}{\|\mathbf{v}_1\|^2}\mathbf{v}_1$

$$= (0,1,1) - \frac{2}{3}(1,1,1) = \left(-\frac{2}{3}, \frac{1}{3}, \frac{1}{3}\right)$$

Step 3. $\mathbf{v}_3 = \mathbf{u}_3 - \text{proj}_{W_2}\mathbf{u}_3 - \dfrac{\langle \mathbf{u}_3, \mathbf{v}_1 \rangle}{\|\mathbf{v}_1\|^2}\mathbf{v}_1 - \dfrac{\langle \mathbf{u}_3, \mathbf{v}_2 \rangle}{\|\mathbf{v}_2\|^2}\mathbf{v}_2$

$$= (0,0,1) - \frac{1}{3}(1,1,1) - \frac{1/3}{2/3}\left(-\frac{2}{3}, \frac{1}{3}, \frac{1}{3}\right) = \left(0, -\frac{1}{2}, \frac{1}{2}\right)$$

Hence,

$$\mathbf{v}_1 = (1,1,1),\ \mathbf{v}_2 = \left(-\frac{2}{3}, \frac{1}{3}, \frac{1}{3}\right),\ \mathbf{v}_3 = \left(0, -\frac{1}{2}, \frac{1}{2}\right)$$

Example 1 solution: Normalization

From the Gram-Schmidt process, we get:

$$\mathbf{v}_1 = (1, 1, 1),\ \mathbf{v}_2 = \left(-\frac{2}{3}, \frac{1}{3}, \frac{1}{3}\right),\ \mathbf{v}_3 = \left(0, -\frac{1}{2}, \frac{1}{2}\right)$$

Hence,

$$\|\mathbf{v}_1\| = \sqrt{3}, \quad \|\mathbf{v}_2\| = \frac{\sqrt{6}}{3}, \quad \|\mathbf{v}_3\| = \frac{1}{\sqrt{2}}$$

So, an orthonormal basis for $\mathbb{R}^3$ is:

$$\mathbf{q}_1 = \frac{\mathbf{v}_1}{\|\mathbf{v}_1\|} = \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right), \quad \mathbf{q}_2 = \frac{\mathbf{v}_2}{\|\mathbf{v}_2\|} = \left(-\frac{2}{\sqrt{6}}, \frac{1}{\sqrt{6}}, \frac{1}{\sqrt{6}}\right),$$

$$\mathbf{q}_3 = \frac{\mathbf{v}_3}{\|\mathbf{v}_3\|} = \left(0, -\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right)$$

Extending orthogonal/orthonormal sets to orthogonal/orthonormal bases

Theorem

If W is a finite-dimensional inner product space, then:

1. *Every orthogonal set of nonzero vectors in W can be enlarged to an orthogonal basis for W.*
2. *Every orthonormal set in W can be enlarged to an orthonormal basis for W.*

Exercises

Part 3: QR-Decomposition

Concept of QR-decomposition (1)

Problem

If:

- *A is an $m \times n$ matrix with linearly independent column vectors,*
- *Q is the matrix that results by applying the Gram-Schmidt process to the column vectors of A,*

what relationship (if any) exists between A and Q?

Concept of QR-decomposition (1)

Problem

If:

- A *is an* $m \times n$ *matrix with linearly independent column vectors,*
- Q *is the matrix that results by applying the Gram-Schmidt process to the column vectors of* A*,*

what relationship (if any) exists between A *and* Q*?*

Let: $A = [\mathbf{u}_1 \mid \mathbf{u}_2 \mid \cdots \mid \mathbf{u}_n]$ and $Q = [\mathbf{q}_1 \mid \mathbf{q}_2 \mid \cdots \mid \mathbf{q}_n]$

By Theorem "Orthogonal basis & orthonormal basis", it can be written:

$$\begin{aligned}
\mathbf{u}_1 &= \langle \mathbf{u}_1, \mathbf{q}_1 \rangle \mathbf{q}_1 + \langle \mathbf{u}_1, \mathbf{q}_1 \rangle \mathbf{q}_1 + \cdots + \langle \mathbf{u}_1, \mathbf{q}_n \rangle \mathbf{q}_n \\
\mathbf{u}_2 &= \langle \mathbf{u}_2, \mathbf{q}_1 \rangle \mathbf{q}_1 + \langle \mathbf{u}_2, \mathbf{q}_1 \rangle \mathbf{q}_1 + \cdots + \langle \mathbf{u}_2, \mathbf{q}_n \rangle \mathbf{q}_n \\
\vdots \quad & \qquad \vdots \qquad\qquad \vdots \qquad\qquad \vdots \qquad\qquad \vdots \\
\mathbf{u}_n &= \langle \mathbf{u}_n, \mathbf{q}_1 \rangle \mathbf{q}_1 + \langle \mathbf{u}_n, \mathbf{q}_1 \rangle \mathbf{q}_1 + \cdots + \langle \mathbf{u}_n, \mathbf{q}_n \rangle \mathbf{q}_n
\end{aligned}$$

Concept of QR-decomposition (2)

This can be written in matrix:

$$[\mathbf{u}_1 \mid \mathbf{u}_2 \mid \cdots \mid \mathbf{u}_n] = [\mathbf{q}_1 \mid \mathbf{q}_2 \mid \cdots \mid \mathbf{q}_n] \begin{bmatrix} \langle \mathbf{u}_1, \mathbf{q}_1 \rangle & \langle \mathbf{u}_2, \mathbf{q}_1 \rangle & \cdots & \langle \mathbf{u}_n, \mathbf{q}_1 \rangle \\ \langle \mathbf{u}_1, \mathbf{q}_2 \rangle & \langle \mathbf{u}_2, \mathbf{q}_2 \rangle & \cdots & \langle \mathbf{u}_n, \mathbf{q}_2 \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle \mathbf{u}_1, \mathbf{q}_n \rangle & \langle \mathbf{u}_2, \mathbf{q}_n \rangle & \cdots & \langle \mathbf{u}_n, \mathbf{q}_n \rangle \end{bmatrix}$$

$$A \quad = \quad Q \quad\quad R$$

Since $\mathbf{q}_j$ is orthogonal to $\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_{j-1}$, we have:

$$R = \begin{bmatrix} \langle \mathbf{u}_1, \mathbf{q}_1 \rangle & \langle \mathbf{u}_2, \mathbf{q}_1 \rangle & \cdots & \langle \mathbf{u}_n, \mathbf{q}_1 \rangle \\ 0 & \langle \mathbf{u}_2, \mathbf{q}_2 \rangle & \cdots & \langle \mathbf{u}_n, \mathbf{q}_2 \rangle \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \langle \mathbf{u}_n, \mathbf{q}_n \rangle \end{bmatrix}$$

This is called the QR-decomposition of matrix A.

Concept of QR-decomposition (3)

Theorem

If A is an $m \times n$ matrix with linearly independent column vectors, then A can be factored as:

$$A = QR$$

where Q is an $m \times n$ matrix with orthonormal column vectors, and R is an $n \times n$ invertible upper triangular matrix.

Remark.

- $Q = [\mathbf{q}_1 \mid \mathbf{q}_2 \mid \cdots \mid \mathbf{q}_n]$ can be obtained from Gram-Schmidt process.
- The matrix R is the matrix as defined previously, which is an upper-triangular matrix whose entries are $\langle \mathbf{u}_i, \mathbf{q}_j \rangle$ for some $i, j \in \{1, 2, \ldots, n\}$.

Example: Finding QR-decomposition

Find a QR-decomposition of:

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

Solution of example

Solution:

Step 1. Find the column vectors of A:

$$\mathbf{u}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix},\ \mathbf{u}_2 = \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix},\ \mathbf{u}_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

Step 2. Apply the Gram-Schmidt process. This gives orthonormal vectors:

$$\mathbf{v}_1 = \begin{bmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \end{bmatrix},\ \mathbf{v}_2 = \begin{bmatrix} -\frac{2}{\sqrt{6}} \\ \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{6}} \end{bmatrix},\ \mathbf{v}_3 = \begin{bmatrix} 0 \\ -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}$$

Step 3. Define matrix R:

$$R = \begin{bmatrix} \langle \mathbf{u}_1, \mathbf{q}_1 \rangle & \langle \mathbf{u}_2, \mathbf{q}_1 \rangle & \langle \mathbf{u}_3, \mathbf{q}_1 \rangle \\ 0 & \langle \mathbf{u}_2, \mathbf{q}_2 \rangle & \langle \mathbf{u}_3, \mathbf{q}_2 \rangle \\ 0 & 0 & \langle \mathbf{u}_3, \mathbf{q}_3 \rangle \end{bmatrix} = \begin{bmatrix} \frac{3}{\sqrt{3}} & \frac{2}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ 0 & \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ 0 & 0 & \frac{1}{\sqrt{2}} \end{bmatrix}$$

Solution of example (*cont.*)

Hence the QR-decomposition is:

$$\begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{3}} & -\frac{2}{\sqrt{6}} & 0 \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{3}{\sqrt{3}} & \frac{2}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ 0 & \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ 0 & 0 & \frac{1}{\sqrt{2}} \end{bmatrix}$$

$$A \quad = \quad Q \quad R$$

Exercises

1. Write the step-by-step procedure of computing QR-decomposition of a matrix.
2.

to be continued...