1 Gram-Schmidt Orthogonalization

Given a basis $\{v_1, \dots, v_m\}$ of a subspace $S \subset \mathbb{R}n$, the Gram-Schmidt process constructs an orthonormal basis $\{q_1, \dots, q_m\}$, i.e., basis where the basis vectors satisfy

$$q_i^T q_j = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{otherwise} \end{cases},$$

of the same subspace S. More precisely, for $k = 1, \dots, m$ the Gram-Schmidt process successively computes an orthonormal basis $\{q_1, \dots, q_k\}$ from $\{v_1, \dots, v_k\}$ such that both bases span the same subspace. The idea is to use orthogonal projection to remove components along the existing basis vectors, leaving an orthogonal set. The geometric idea is illustrated in Figure 1.

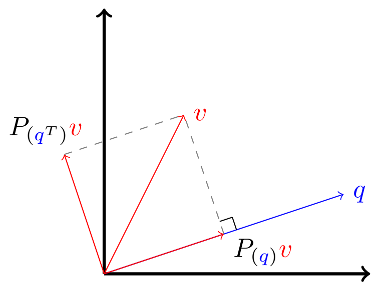

Figure 1: The projectors $P_{(q)} = qq^T/(q^Tq)$ and $P_{(q^T)} = I - P_{(q)}$ decompose the vector v into the component $P_{(q)}v$ along q, and the orthogonal component $P_{(q^T)}v$.

The steps of the Gram-Schmidt process are described next.

$k = 1$. If $k = 1$, then we need to find a vector q_1 with $q_1^T q_1 = 1$ such that

$$\text{span}\{q_1\} = \text{span}\{v_1\}.$$

The vector q_1 is obtained by normalizing v_1:

$$q_1 = v_1/\|v_1\|_2.$$

$k = 2$. Given q_1 we want to compute q_2 such that $q_1^T q_2 = 0$, $q_2^T q_2 = 1$, and

$$\text{span}\{q_1, q_2\} = \text{span}\{v_1, v_2\}.$$

First note that since $\text{span}\{q_1\} = \text{span}\{v_1\}$ we have $\text{span}\{v_1, v_2\} = \text{span}\{q_1, q_2\}$. Moreover, by the Fundamental Theorem of Linear Algebra we can write v_2 as the sum of vector in $\text{span}\{q_1\} = (Q_1)$, where Q_1 is the matrix $Q_1 = (q_1) \in \mathbb{R}n \times 1$, and a vector in the orthogonal complement of (Q_1). We can use projections to express these vectors. The projection onto (Q_1)

is given by $P_{(Q_1)} = Q_1(Q_1^T Q_1)^{-1} Q_1^T$. Since $q_1^T q_1 = 1$, $Q_1^T Q_1 = 1$ and the projection is given by

$$P_{(Q_1)} = Q_1 Q_1^T.$$

Hence,

$$v_2 = Q_1 Q_1^T v_2 + (I - Q_1 Q_1^T) v_2.$$

Since $Q_1 Q_1^T v_2 \in (Q_1) = \text{span}\{q_1\}$ we have

$$\text{span}\{q_1, v_2\} = \text{span}\{q_1, (I - Q_1 Q_1^T) v_2\}.$$

The vector

$$\widetilde{q}_2 = (I - Q_1 Q_1^T) v_2 = v_2 - (q_1^T v_2) q_1$$

is orthogonal to q_1. We just need to normalize it to obtain

$$q_2 = \widetilde{q}_2 / \|\widetilde{q}_2\|_2.$$

We have

$$\text{span}\{v_1, v_2\} = \text{span}\{q_1, v_2\} = \text{span}\{q_1, (I - Q_1 Q_1^T) v_2\} = \text{span}\{q_1, q_2\}$$

$k > 2$. Given $q_1, \ldots, q_{k-1}$ with

$$q_i^T q_j = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{otherwise} . \end{cases}$$

and $\text{span}\{q_1, \ldots, q_{k-1}\} = \text{span}\{v_1, \ldots, v_{k-1}\}$, we want to compute q_k such that $q_j^T q_k = 0$, $j = 1, \ldots, k-1$, $q_k^T q_k = 1$, and

$$\text{span}\{q_1, \ldots, q_{k-1}, q_k\} = \text{span}\{v_1, \ldots, v_{k-1}, v_k\}.$$

Since $\text{span}\{q_1, \ldots, q_{k-1}\} = \text{span}\{v_1, \ldots, v_{k-1}\}$ we have

$$\text{span}\{v_1, \ldots, v_{k-1}, v_k\} = \text{span}\{q_1, \ldots, q_{k-1}, v_k\}.$$

By the Fundamental Theorem of Linear Algebra we can write v_k as the sum of vector in $\text{span}\{q_1, \ldots, q_{k-1}\} = (Q_{k-1})$, where Q_{k-1} is the matrix $Q_{k-1} = (q_1, \ldots, q_{k-1}) \in \mathbb{R}n \times k-1$, and a vector in the orthogonal complement of (Q_{k-1}). We can use projections to express these vectors. The projection onto (Q_{k-1}) is given by $P_{(Q_{k-1})} = Q_{k-1}(Q_{k-1}^T Q_{k-1})^{-1} Q_{k-1}^T$. Since the columns $q_1, \ldots, q_{k-1}$ of Q_{k-1} are orthonormal, $Q_{k-1}^T Q_{k-1} = I$ and the projection is given by

$$P_{(Q_{k-1})} = Q_{k-1} Q_{k-1}^T.$$

Hence,

$$v_k = Q_{k-1} Q_{k-1}^T v_k + (I - Q_{k-1} Q_{k-1}^T) v_k.$$

Since $Q_1 Q_1^T v_2 \in (Q_1) = \text{span}\{q_1\}$ we have

$$\text{span}\{q_1, \ldots, q_{k-1}, v_2\} = \text{span}\{q_1, \ldots, q_{k-1}, (I - Q_{k-1} Q_{k-1}^T) v_k\}.$$

The vector

$$\widetilde{q}_k = (I - Q_{k-1}Q_{k-1}^T)v_k = v_k - \sum_{j=1}^{k-1}(q_j^T v_k)q_j$$

is orthogonal to $q_1, \ldots, q_{k-1}$. We just need to normalize it to obtain

$$q_k = \widetilde{q}_k / \|\widetilde{q}_k\|_2.$$

We have

$$\begin{aligned}\operatorname{span}\{v_1, \ldots, v_{k-1}, v_k\} &= \operatorname{span}\{q_1, \ldots, q_{k-1}, v_k\} = \operatorname{span}\{q_1, \ldots, q_{k-1}, (I - Q_{k-1}Q_{k-1}^T)v_k\} \\ &= \operatorname{span}\{q_1, \ldots, q_{k-1}, q_k\}.\end{aligned}$$

We use the Gram-Schmidt method to compute orthonormal eigenvectors, i.e., to compute orthonormal bases for the eigenspaces $\mathcal{N}(\lambda_j I - A)$.

In Example **??** we have shown that the matrix

$$A = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$$

has eigenvalues $\lambda_1 = 0$, $\lambda_2 = 0$, $\lambda_3 = 3$. The corresponding eigenspaces, i.e, the nullspaces $\mathcal{N}(0I - A)$ and $\mathcal{N}(3I - A)$ are

$$\begin{aligned}\mathcal{N}(0I - A) &= \operatorname{span}\Big\{ \begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} \Big\}, \\ \mathcal{N}(3I - A) &= \operatorname{span}\Big\{ \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \Big\}.\end{aligned}$$

Furthermore, we have shown that

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} = \underbrace{\begin{pmatrix} -1 & -1 & 1 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix}}_{=V} \underbrace{\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 3 \end{pmatrix}}_{=\Lambda} \underbrace{\begin{pmatrix} -1/3 & 2/3 & -1/3 \\ -1/3 & -1/3 & 2/3 \\ 1/3 & 1/3 & 1/3 \end{pmatrix}}_{=V^{-1}}.$$

The matrix V of eigenvectors is invertible, but not orthonormal. This is due to the fact that we have computed bases of the eigenspaces $\mathcal{N}(0I - A)$ and $\mathcal{N}(3I - A)$, but not orthonormal bases.

We can do this now using Gram-Schmidt. To compute an orthonormal basis for $\mathcal{N}(0I - A)$ we proceed as follows. Let $v_1 = (-1, 1, 0)^T$ and $v_2 = (-1, 0, 1)^T$.

An orthonormal basis is obtained by computing

$$q_1 = v_1/\|v_1\|_2 = -1$$
$$1$$
$$0/\sqrt{2},$$
$$\widetilde{q}_2 = v_2 - (v_2^T q_1)\, q_1 = -1$$
$$0$$
$$1 - \frac{1}{2} - 1$$
$$1$$
$$0 = -1/2$$
$$-1/2$$
$$1,$$
$$q_2 = \widetilde{q}_2/\|\widetilde{q}_2\| = \frac{1}{\sqrt{6}} - 1$$
$$-1$$
$$2.$$

To compute an orthonormal basis for $\mathcal{N}(3I - A)$ we just need to normalize the original basis vector. The normalized basis vector is

$$q_3 = \frac{1}{\sqrt{3}} 111.$$

It is easy to verify that the vectors q_1, q_2, q_3 are orthogonal.

The vectors q_1, q_2 are eigenvectors corresponding to the eigenvalue 0 and the vector q_3 is an eigenvectors corresponding to the eigenvalue 3. Hence

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \underbrace{\begin{pmatrix} -1/\sqrt{2} & -1//\sqrt{6} & 1/\sqrt{3} \\ 1/\sqrt{2} & -1//\sqrt{6} & 1/\sqrt{3} \\ 0 & 2/\sqrt{6} & 1/\sqrt{3} \end{pmatrix}}_{=Q} = \underbrace{\begin{pmatrix} -1/\sqrt{2} & -1//\sqrt{6} & 1/\sqrt{3} \\ 1/\sqrt{2} & -1//\sqrt{6} & 1/\sqrt{3} \\ 0 & 2/\sqrt{6} & 1/\sqrt{3} \end{pmatrix}}_{=Q} \underbrace{\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 3 \end{pmatrix}}_{=\Lambda}.$$

Since the matrix Q is orthogonal, $Q^{-1} = Q^T$ and we have

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} = \underbrace{\begin{pmatrix} -1/\sqrt{2} & -1/\sqrt{6} & 1/\sqrt{3} \\ 1/\sqrt{2} & -1/\sqrt{6} & 1/\sqrt{3} \\ 0 & 2/\sqrt{6} & 1/\sqrt{3} \end{pmatrix}}_{=Q} \underbrace{\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 3 \end{pmatrix}}_{=\Lambda} \underbrace{\begin{pmatrix} -1/\sqrt{2} & 1/\sqrt{2} & 0 \\ -1/\sqrt{6} & -1/\sqrt{6} & 2/\sqrt{6} \\ 1/\sqrt{3} & 1/\sqrt{3} & 1/\sqrt{3} \end{pmatrix}}_{=Q^T}.$$

If we use Matlab to compute the eigendecomposition of A we obtain

```
>> A = ones(3,3);
>> [Q,Lambda]=eig(A);
```

```
>> Q

Q =

    0.4082    0.7071    0.5774
    0.4082   -0.7071    0.5774
   -0.8165         0    0.5774

>> Lambda

Lambda =

   -0.0000         0         0
         0         0         0
         0         0    3.0000
```

Note that the first column in the matrix `Q` computed by Matlab is $-q_2$ and the second column in the matrix `Q` computed by Matlab is $-q_1$. Thus, the first two columns in the matrix `Q` computed by Matlab are just another orthonormal basis for $\mathcal{N}(0I - A)$.