QR Decomposition using Gram-Schmidt Orthogonalization

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Abstract A very quick and easy to understand introduction to Gram-Schmidt Orthogonalization (Orthonormalization) and how to obtain QR decomposition of a matrix using it.

Aim Given a basis $\mathbb{B}$ of a vector subspace **V** spanned by vectors $\{v_1, v_2, \ldots, v_n\}$ it is required to find an orthonormal basis $\{q_1, q_2, \ldots, q_n\}$ (A basis that is orthogonal with unit length of constituent vectors). Thus,

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

Proof. Note that $\text{span}\{v_1, v_2, \ldots, v_n\} = \text{span}\{q_1, q_2, \ldots, q_n\}$ (successive spanning)
Lets start with one vector v_1, normalize this to obtain vector q_1 as

$$q_1 = \frac{v_1}{\|v_1\|} \tag{1}$$

Now, lets include another vector, v_2 to the picture [1]. We have already obtained q_1, now we need q_2, which can be obtained by normalizing a vector that is orthogonal to $v_1(q_1)$. Suppose, this vector is $\tilde{v}_2$. By triangle law of vectors, it can be seen that

$$\tilde{v}_2 = v_2 - v_1$$

But, to be more formal in line with the algorithm we write $\tilde{v}_2$ as

$$\tilde{v}_2 = v_2 - \text{proj}_{v_1}(v_2) = v_2 - \langle v_2, q_1 \rangle q_1 \tag{2}$$

and,

$$q_2 = \frac{\tilde{v}_2}{\|\tilde{v}_2\|}$$

where, $\langle a, b \rangle = a^T b$ is the inner product.
Going one step further we include v_3 and proceed on similar lines to obtain $\tilde{v}_3$ as

$$\tilde{v}_3 = v_3 - \langle v_3, q_1 \rangle q_1 - \langle v_3, q_2 \rangle q_2,\ q_3 = \tilde{v}_3 / \|\tilde{v}_3\| \tag{3}$$

Similarly,

$$\tilde{v}_4 = v_4 - \langle v_4, q_1 \rangle q_1 - \langle v_4, q_2 \rangle q_2 - \langle v_4, q_3 \rangle q_3,\ q_3 = \tilde{v}_4 / \|\tilde{v}_4\| \tag{4}$$

[1] This is a preliminary version of the document, a more elaborate document will be made available soon.

So, this process continues and we are in a position to write the expression for $\tilde{v}_\mathrm{n}$

$$\tilde{v}_\mathrm{n} = v_\mathrm{n} - \langle v_\mathrm{n}, q_1 \rangle\, q_1 - \langle v_\mathrm{n}, q_2 \rangle\, q_2 - \cdots - \langle v_\mathrm{n}, q_\mathrm{n-1} \rangle\, q_\mathrm{n-1},\ q_n = \tilde{v}_n / \left\| \tilde{v}_n \right\| \tag{5}$$

In compact form,

$$\tilde{v}_\mathrm{n} = v_\mathrm{n} - \sum_{i=0}^{n-1} \langle v_\mathrm{n}, q_\mathrm{i} \rangle\, q_\mathrm{i}$$

□

Hence, we have obtained an orthonormal basis from a regular basis for the vector subspace **V**.

Obtaining QR decomposition

Now, let us rearrange the equations (1) to (5) in terms of v's only

$$\begin{aligned}
v_1 &= \left\| v_1 \right\| q_1 && (6)\\
v_2 &= \langle v_2, q_1 \rangle\, q_1 + \tilde{v}_2 = \langle v_2, q_1 \rangle\, q_1 + \left\| \tilde{v}_2 \right\| q_2 && (7)\\
v_3 &= \langle v_3, q_1 \rangle\, q_1 + \langle v_3, q_2 \rangle\, q_2 + \tilde{v}_3 = \langle v_3, q_1 \rangle\, q_1 + \langle v_3, q_2 \rangle\, q_2 + \left\| \tilde{v}_3 \right\| q_3 && (8)\\
v_4 &= \langle v_4, q_1 \rangle\, q_1 + \langle v_4, q_2 \rangle\, q_2 + \langle v_4, q_3 \rangle\, q_3 + \left\| \tilde{v}_4 \right\| q_4 = && (9)
\end{aligned}$$

$$\vdots$$

$$v_n = \langle v_\mathrm{n}, q_1 \rangle\, q_1 + \langle v_\mathrm{n}, q_2 \rangle\, q_2 + \cdots + \langle v_\mathrm{n-1}, q_\mathrm{n-1} \rangle\, q_\mathrm{n-1} + \left\| \tilde{v}_\mathrm{n} \right\| q_\mathrm{n} \tag{10}$$

And rewrite these equations in the matrix form, we get

$$\begin{bmatrix} v_1 & v_2 & \dots & v_\mathrm{n} \end{bmatrix} = \begin{bmatrix} q_1 & q_2 & \dots & q_\mathrm{n} \end{bmatrix} \begin{bmatrix} \left\| v_1 \right\| & \langle v_2, q_1 \rangle & \langle v_3, q_1 \rangle & \dots & \langle v_\mathrm{n}, q_1 \rangle \\ 0 & \left\| \tilde{v}_2 \right\| & \langle v_3, q_2 \rangle & \dots & \langle v_\mathrm{n}, q_2 \rangle \\ 0 & 0 & \left\| \tilde{v}_3 \right\| & \dots & \langle v_\mathrm{n}, q_3 \rangle \\ 0 & 0 & 0 & \ddots & \vdots \\ 0 & 0 & 0 & \left\| \tilde{v}_\mathrm{n-1} \right\| & \langle v_\mathrm{n-1}, q_\mathrm{n-1} \rangle \\ 0 & 0 & 0 & 0 & \left\| \tilde{v}_\mathrm{n} \right\| \end{bmatrix} \tag{11}$$

$$\text{or}, V = QR \tag{12}$$