Gram-Schmidt Orthogonalization and QR Decomposition

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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. A basic background in linear algebra is assumed.

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,

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

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

$$q_1 = \frac{v_1}{\|v_1\|}$$
(1)

Now, lets include another vector, v_2 to the picture (See Fig. 1)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 lines with the algorithm we write \tilde{v}_2 as

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

and,

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

where, $\langle a, b \rangle = a^{\mathrm{T}}b$ is the inner product.

Please contact for any clarifications, or found errors. Thanks!

¹This is an improved version of the document with the figures included, it would have been better if a successive series of figures were included showing the process step by step. An animation of the GS process can be found on Wikipedia here: https://en.wikipedia.org/wiki/Gram-Schmidt_process

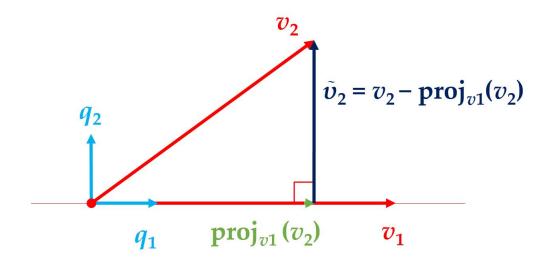


Figure 1: Obtaining an orthonormal basis-2D case

Going one step further we include v_3 and proceed on similar lines to obtain \tilde{v}_3 as

$$\tilde{v}_{3} = v_{3} - \operatorname{proj}_{q_{1}}(v_{3}) - \operatorname{proj}_{q_{2}}(v_{3})
= v_{3} - \langle v_{3}, q_{1} \rangle q_{1} - \langle v_{3}, q_{2} \rangle q_{2}
q_{3} = \tilde{v}_{3} / \|\tilde{v}_{3}\|$$
(3)

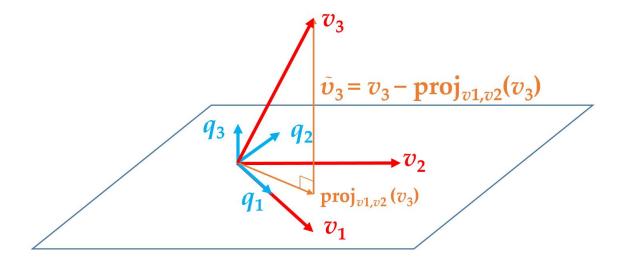


Figure 2: Obtaining an orthonormal basis-3D case

Similarly,

$$\tilde{v}_4 = v_4 - \langle v_4, q_1 \rangle \, q_1 - \langle v_4, q_2 \rangle \, q_2 - \langle v_4, q_3 \rangle \, q_3, \ q_4 = \tilde{v}_4 / \| \tilde{v}_4 \| \tag{4}$$

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

$$\tilde{v}_n = v_n - \langle v_n, q_1 \rangle q_1 - \langle v_n, q_2 \rangle q_2 - \dots - \langle v_n, q_{n-1} \rangle q_{n-1}, \ q_n = \tilde{v}_n / \|\tilde{v}_n\|$$
(5)

In compact form,

$$ilde{v}_n = v_n - \sum_{i=0}^{n-1} \left< v_n, q_{\mathrm{i}} \right> q_{\mathrm{i}}$$

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

$$v_1 = \|v_1\| q_1 \tag{6}$$

$$v_2 = \langle v_2, q_1 \rangle q_1 + \tilde{v}_2 = \langle v_2, q_1 \rangle q_1 + \| \tilde{v}_2 \| q_2$$
(7)

$$v_3 = \langle v_3, q_1 \rangle q_1 + \langle v_3, q_2 \rangle q_2 + \tilde{v}_3 = \langle v_3, q_1 \rangle q_1 + \langle v_3, q_2 \rangle q_2 + \|\tilde{v}_3\| q_3$$
(8)

$$v_4 = \langle v_4, q_1 \rangle q_1 + \langle v_4, q_2 \rangle q_2 + \langle v_4, q_3 \rangle q_3 + \| \tilde{v}_4 \| q_4$$
(9)

$$\vdots$$

$$v_n = \langle v_n, q_1 \rangle q_1 + \langle v_n, q_2 \rangle q_2 + \dots + \langle v_{n-1}, q_{n-1} \rangle q_{n-1} + \|\tilde{v}_n\| q_n \qquad (10)$$

And rewrite these equations in the matrix form, we get

$$\begin{bmatrix} v_1 & v_2 & \dots & v_n \end{bmatrix} = \begin{bmatrix} q_1 & q_2 & \dots & q_n \end{bmatrix} \begin{bmatrix} \|v_1\| & \langle v_2, q_1 \rangle & \langle v_3, q_1 \rangle & \dots & \langle v_n, q_1 \rangle \\ 0 & \|\tilde{v}_2\| & \langle v_3, q_2 \rangle & \dots & \langle v_n, q_2 \rangle \\ 0 & 0 & \|\tilde{v}_3\| & \dots & \langle v_n, q_3 \rangle \\ 0 & 0 & 0 & \ddots & \vdots \\ 0 & 0 & 0 & \|\tilde{v}_{n-1}\| & \langle v_{n-1}, q_{n-1} \rangle \\ 0 & 0 & 0 & 0 & \|\tilde{v}_n\| \end{bmatrix}$$
(11)
or, $V = QR$

Thus, we have obtained the QR decomposition of the matrix *A* starting from the Gram-Schmidt process, where *Q* is an orthonormal matrix and *R* is an upper triangular matrix.