QR Decomposition

- The QR decomposition is perhaps the most important algorithmic idea in numerical linear algebra.
 - ◇ Suppose $A \in \mathbb{R}^{m \times n}$, $m \ge n$, and suppose rank (A) = n (i.e., suppose A has linearly independent columns).
 - \diamond The matrix A can always be decomposed as the product

$$A = QR, \tag{0.1}$$

where $Q = R^{m \times m}$ is an orthogonal matrix (i.e., $Q^T Q = I_m$), and $R \in R^{m \times n}$ is a matrix of the form $R = \begin{bmatrix} R_1 \\ 0 \end{bmatrix}$ with $R_1 \in R^{n \times n}$ an upper triangular matrix.

 \triangleright Because of the zeros at the lower part of R, the decomposition can be simplified as

$$A = Q_1 R_1 \tag{0.2}$$

where $Q_1 \in \mathbb{R}^{m \times n}$ is made of the first *n* columns of *Q* and satisfies $Q_1^T Q_1 = I_n$ (but it is not orthogonal.) This is called the *reduced QR factorization* of *A*.

- Suppose A = QR. Then the system Ax = b can be solved from the triangular system $Rx = Q^T b$. This is an excellent method for solving linear systems, but it is *not* the standard method for such problems.
 - ♦ Gaussian elimination requires only half as many numerical operations in the QR decomposition.
- The QR decomposition can also be used in solving least squares problems and eigenvalue problems.

Gram-Schmidt Orthogonalization

- Given a set of linearly independent column vectors {v₁,..., v_n} ⊂ R^m (m ≥ n), these vectors span an n-dimensional vector subspace of R^m. We could construct an orthonormal set of vectors {q₁,..., q_n} that spans the same subspace. The well-known Gram-Schmidt process provides a recipe for accomplishing this:
 - \diamond Set $w_1 := v_1$.
 - \diamond Set, in general, for $j = 2, \ldots, n$

$$w_j := v_j - \sum_{i=1}^{j-1} \frac{\langle w_i, v_j \rangle}{\langle w_i, w_i \rangle} w_i$$

- ▷ It is really to be verified that $\langle w_i, w_j \rangle = 0$ for $i \neq j$, and that $w_j \neq 0$.
- \triangleright If we define $q_j := \frac{w_j}{\|w_j\|_2}$, then $\langle q_i, q_j \rangle = \delta_{ij}$.
- The above relationship may be rewritten as

$$v_1 = w_1;$$

$$v_j = w_j + \sum_{i=1}^{j-1} \frac{\langle w_i, v_j \rangle}{\langle w_i, w_i \rangle} w_i.$$

• In matrix form, we may record the above relationship as

$$\begin{bmatrix} v_1, \dots, v_n \end{bmatrix} = \begin{bmatrix} v_1, \dots, v_n \end{bmatrix} \begin{bmatrix} 1 & \frac{\langle w_1, v_2 \rangle}{\langle w_i, w_1 \rangle} & \frac{\langle w_1, v_3 \rangle}{\langle w_1, w_1 \rangle} \\ 0 & 1 & \frac{\langle w_2, v_3 \rangle}{\langle w_2, w_2 \rangle} \\ 0 & 0 & 1 \\ \vdots & \vdots & \ddots \\ 0 & 0 & 0 & \dots & 1 \end{bmatrix}.$$

That is, $V = W\tilde{R}$.

- \diamond Let $D := \text{diag} \left\{ \frac{1}{\|w_1\|}, \dots, \frac{1}{\|w_n\|} \right\}$ denote the scaling factors.
- \diamond Then $V = WDD^{-1}\tilde{R} = Q_1R_1$ where $Q_1 := WD$ and $R_1 := D^{-1}\tilde{R}$.
- For our consideration, identify the matrix V as our original matrix A.
 - ◊ The Gram-Schmidt process offers a numerical procedure to compute the QR decomposition.
 - ◊ In practice, the sequence of Gram-Schmidt calculations turns to be numerically unstable. Fortunately, there are better way.
 - \diamond The insight we obtained from the Gram-Schmidt process is that the columns of A and columns of Q generate the same range space.