From (7.5) it is evident that an appropriate definition for the coefficients r_{ij} in the numerators of (7.6) is

$$r_{ij} = q_i^* a_j \qquad (i \neq j). \tag{7.7}$$

The coefficients r_{jj} in the denominators are chosen for normalization:

$$|r_{jj}| = \Big\| a_j - \sum_{i=1}^{j-1} r_{ij} q_i \Big\|_2 . \tag{7.8}$$

Note that the sign of r_{jj} is not determined. Arbitrarily, we may choose $r_{jj} > 0$, in which case we shall finish with a factorization $A = \hat{Q}\hat{R}$ in which $\hat{R}$ has positive entries along the diagonal.

The algorithm embodied in (7.6)–(7.8) is the Gram–Schmidt iteration. Mathematically, it offers a simple route to understanding and proving various properties of QR factorizations. Numerically, it turns out to be unstable because of rounding errors on a computer. To emphasize the instability, numerical analysts refer to this as the *classical Gram–Schmidt iteration*, as opposed to the *modified Gram–Schmidt iteration*, discussed in the next lecture.

Algorithm 7.1. Classical Gram–Schmidt (unstable)

for $j = 1$ **to** n
  $v_j = a_j$
  for $i = 1$ **to** $j - 1$
    $r_{ij} = q_i^* a_j$
    $v_j = v_j - r_{ij} q_i$
  $r_{jj} = \|v_j\|_2$
  $q_j = v_j / r_{jj}$

Existence and Uniqueness

All matrices have QR factorizations, and under suitable restrictions, they are unique. We state first the existence result.

Theorem 7.1. *Every $A \in \mathbb{C}^{m\times n}$ $(m \geq n)$ has a full QR factorization, hence also a reduced QR factorization.*

Proof. Suppose first that A has full rank and that we want just a reduced QR factorization. In this case, a proof of existence is provided by the Gram–Schmidt algorithm itself. By construction, this process generates orthonormal columns of $\hat{Q}$ and entries of $\hat{R}$ such that (7.4) holds. Failure can occur only if at some step, v_j is zero and thus cannot be normalized to produce q_j.