A Gram-Schmidt Puzzle

Let $A \in \mathbb{R}^{m \times n}$ have linearly independent columns $a_1, a_2, \ldots, a_n$. There are many ways to implement the Gram–Schmidt process, which gives the thin QR factorization of A. Recall that in exact arithmetic the *thin* QR factorization yields $Q \in \mathbb{R}^{m \times n}$ with $Q^T Q = I$ and an upper triangular $R \in \mathbb{R}^{n \times n}$, satisfying $A = QR$. You may want to refer to our notes on Classical (CGS) and Modified (MGS) Gram-Schmidt methods.

Some implementations generate R row-by-row, some column-by-column, some emphasize matrix-vector products, some vector-matrix products, etc., etc. In exact arithmetic, all implementations give exactly the same results. But every implementation can be classified as either CGS or MGS.

The difference appears in the presence of rounding errors and for $n > 2$. All of the CGS implementations give (essentially) the same results as the other CGS implemtations. All of the MGS implementations give (essentially) the same results as the other MGS implementations.

But between CGS and MGS there can be – and usually is – a big difference.

The following pseudo-code is either CGS or MGS (I'm not telling which), and can be changed from one to the other with the alteration of *exactly one character*.

Your challenge is to (i) decide whether it is a CGS or an MGS code, and then to (ii) specify which character needs to be altered to morph it into the other (give the line number and the character change). [Awkwardness in the code gives a clue...]

1 for k=1:n,
2 $\quad u = a_k$
3 $\quad v = a_k$
4 $\quad$ for j = 1:k-1,
5 $\qquad r_{jk} = q_j^T u$
6 $\qquad v = v - r_{jk} q_j$
7 $\quad$ end j-loop
8 $\quad r_{kk} = \|v\|_2$
9 $\quad q_k = v / r_{kk}$
0 end k-loop

You should also (iii) show that in exact arithmetic (no rounding errors) the two versions produce the exact same results (same R and Q).

When rounding errors are made the columns of Q are not exactly orthogonal, so the computed Q does not satisfy $Q^T Q = I$. Rounding error analyses elucidating the differences between the methods have been done, but are rather subtle and beyond the scope of this course.