## Classical Gram-Schmidt vs Modified Gram-Schmidt

Let  $A \in \mathbb{R}^{m \times n}$ , with  $m \ge n$ , and let A have n linearly independent columns  $a_1, a_2, \ldots, a_n$ . There are many ways to implement the Gram-Schmidt process. Here are two *very* different implementations:

Classical	Modified
for $k=1:n$ ,	for $k=1:n$ ,
$w = a_k$	$w = a_k$
for $j = 1:k-1$ ,	for $j=1:k-1$ ,
$r_{jk} = q_j^t w$	
end	$r_{jk} = q_j^t w$
for $j = 1:k-1$ ,	$w = w - r_{jk}q_j$
$w = w - r_{jk}q_j$	
end	end
$r_{kk} =   w  _2$	$r_{kk} =   w  _2$
$q_k = w/r_{kk}$	$q_k = w/r_{kk}$
end	end

Please study the pseudocode above carefully. In exact arithmetic, these two methods generate exactly the same output. Before going on think about why, in the presence of rounding errors, they behave so differently.

In classical Gram–Schmidt (CGS) we compute the (signed) lengths of the orthogonal projections of  $w=a_k$  onto  $q_1,q_2,\ldots,q_{k-1}$ , and then subtract those projections (and the rounding errors) from w. If  $Q_{k-1}=[q_1,q_2,\ldots,q_{k-1}]$ , then the orthogonal projector onto  $\operatorname{ColSp}(Q_{k-1})$  is  $P=Q_{k-1}(Q_{k-1}^tQ_{k-1})^{-1}Q_{k-1}^t$ . If  $Q_{k-1}$  has orthonormal columns, then  $P=Q_{k-1}Q_{k-1}^t$ :

$$w = (I - Q_{k-1}Q_{k-1}^t)a_k.$$

But because of rounding errors,  $Q_{k-1}$  does not have truly orthogonal columns. In modified Gram-Schmidt (MGS) we compute the length of the projection of  $w = a_k$  onto  $q_1$  and subtract that projection (and the rounding errors) from w. Next we compute the length of the projection of the *computed* w onto  $q_2$  and subtract that projection (and the rounding errors) from w, and so on, but always orthogonalizing against the **computed version** of w. Evaluated from right to left:

$$w = (I - q_{k-1}q_{k-1}^t) \dots (I - q_2q_2^t)(I - q_1q_1^t)a_k.$$

If the computed  $Q_{k-1}^t Q_{k-1} = I + E$ , then this is very nearly the same w that would be computed by

$$w = (I - Q_{k-1}(Q_{k-1}^t Q_{k-1})^{-1} Q_{k-1}^t) a_k$$

where we replace  $(Q_{k-1}^t Q_{k-1})^{-1}$  by I - E, and is much "more orthogonal" to  $Q_{k-1}$  than the CGS w.