Two QR Factorizations

We compare two techniques for QR factorizations of a full-rank matrix $A \in \mathbb{R}^{m \times n}$, with $m \geq n$. While there are a few other methods available for use, we will talk here about the modified Gram-Schmidt process (MGS), and the Householder QR factorization (HQR).

**MGS thin QR factorization:**

$$A = QR,$$

where $Q \in \mathbb{R}^{m \times n}$ satisfies $Q^tQ = I$ and $R \in \mathbb{R}^{n \times n}$ is upper triangular. The cost is $2mn^2 + O(mn)$ flops. If $A$ is overwritten by $Q$, then only $\frac{1}{2}n^2 + O(n)$ words of memory are required. If $\tilde{Q}$ and $\tilde{R}$ are the computed versions of $Q$ and $R$, then there exists $\delta A \in \mathbb{R}^{m \times n}$ with $A + \delta A = \tilde{Q}\tilde{R}$, where $\|\delta A\| = \|A\|O(\mu)$, and $\|\tilde{Q}^t\tilde{Q} - I\| = \kappa(A)O(\mu)$.

**HQR factored-Q full QR factorization:**

$$A = QR,$$

where $Q \in \mathbb{R}^{m \times m}$ satisfies $Q^tQ = QQ^t = I$ and $R \in \mathbb{R}^{m \times n}$ is upper triangular. We say “factored” here because HQR does not produce $Q$, but instead produces $u_1, u_2, \ldots, u_n$, where $H_k = H(u_k)$ and $Q = H_1H_2\cdots H_s$. The cost is $2mn^2 - \frac{2}{3}n^3 + O(mn)$ flops. If $A$ is overwritten by $u_1, u_2, \ldots, u_n$ and the strict upper triangle of $R$ (for example), then only $O(n)$ words of memory are required. If $\tilde{R}$ is the computed version of $R$ and $\tilde{Q}$ is the exactly formed $Q$ matrix defined by the computed $u_1, u_2, \ldots, u_n$, then there exists $\delta A \in \mathbb{R}^{m \times n}$ with $A + \delta A = \tilde{Q}\tilde{R}$, where $\|\delta A\| = \|A\|O(\mu)$.

**HQR explicit-Q full QR factorization:**

Let’s say $Q = [Q_1 \quad Q_2]$, where $Q_1 \in \mathbb{R}^{m \times n}$. If only $Q_1$, is needed, then the flop requirements are doubled, to $4mn^2 - \frac{4}{3}n^3$, and the memory requirements are $\frac{1}{2}mn + O(n)$. If $\tilde{Q}_1$ is the computed version of $Q_1$, then $\|\tilde{Q}_1^t\tilde{Q}_1 - I\| = O(\mu)$. If all of $Q$ is explicitly required, then the flop requirements become $4m^2n - 2mn^2 + \frac{2}{3}n^3$ and memory requirements become $O(m^2)$ words. If $\tilde{Q}$ is that computed version of $Q$, then $\|\tilde{Q}^t\tilde{Q} - I\| = O(\mu)$.

**MGS & HQR**

both represent a orthonormal basis (O.B.) for ColSp($A$). In exact arithmetic, each column of $Q$ from MGS is $\pm$ the corresponding column of $Q_1$ from HQR. In other words, the thin part of the full QR is the thin QR. MGS computes $Q_1$ faster, but explicit HQR gives a “more orthogonal” basis. Implemented with care, both methods are backward stable for (LS).