Lecture notes: Householder transformations
Friday September 15, 2017

These notes are not a substitute for class attendance. Their main purpose is to provide a lecture overview summarizing the topics covered.

Reading: Trefethen & Bau III, Lecture 10

Even though the modified Gram-Schmidt procedure is more stable than the standard Gram-Schmidt algorithm, there is a procedure that performs even more stably than modified Gram-Schmidt: triangularization via Householder reflections.
First some preliminaries:

Lemma 1. *Let $P \in \mathbb{C}^{n\times n}$ be an orthogonal projection matrix. Then $I - 2P$ is Hermitian, unitary, and involutory.*

This result implies that operations using $I - 2P$ are stably, mainly since they are unitary. The special case of P a rank-1 orthogonal projection matrix is called a *Householder reflection*. Any rank-1 orthogonal projector is defined by a single vector: the range of P. Let $v \in \mathbb{C}^n$ be a unit vector in the range of P. Then $P = vv^*$, and

$$I - 2P = I - 2vv^*. \tag{1}$$

Note in particular that application of $I - 2P$ on a vector does note require formation of the full Householder reflection matrix.
The main utility of Householder reflections is the ability to unitarily transform an arbitrary nontrivial vector $x \in \mathbb{C}^n$ to a new vector pointing in the direction of the cardinal vector e_1, defined by

$$e_1 = (1, 0, \ldots, 0)^T \in \mathbb{C}^n.$$

More precisely, for any $\theta \in [0, 2\pi)$, we seek to define $v = v(x)$ so that the resulting Householder reflection accomplishes

$$(I - 2P)x = \|x\| e^{i\theta} e_1$$

One can see that we can accomplish this by defining

$$v = \frac{x - \|x\| e^{i\theta} e_1}{\|x - \|x\| e^{i\theta} e_1\|} \tag{2}$$

The choice of θ can be arbitrary, but numerical algorithms are generally more stable when such operations transform vectors in “large” ways. I.e., for stability we want

$$\|x - (I - 2P)x\| = 2\|Px\|$$

to be as large as possible. A computation shows that this happens when

$$e^{i\theta} = -\frac{x_1}{|x_1|}, \tag{3}$$

where x_1 is the first element in the vector x. Then, given a nontrivial x, the full Householder reflection procedure defines $Q = I - 2P$ via (1), (2), and (3).

How is this useful for QR factorizations? A Gram-Schmidt procedure for computing QR factorizations starts with A and attempts to transform it into a unitary Q via column operations, i.e., it performs

$$A \to AR^{-1} = Q$$

In constrast, a Householder transformations procedure for computing a QR factorization starts with A and attempts to transform it into an upper triangular matrix via row operations, i.e., it performs

$$A \to Q^* A = R$$

This triangularization is accomplished via Householder reflections, where a subset of a column is reflected to the direction e_1. At step k of the procedure, we have the following block structure for a transformed A:

$$A = \begin{bmatrix} \widetilde{R}_{k-1} & \widehat{R}_{k-1} \\ 0_{k-1\times n-k+1} & \widetilde{A}_{k-1} \end{bmatrix} \in \mathbb{C}^{m\times n}, \quad \widetilde{R}_{k-1} \in \mathbb{C}^{(k-1)\times(k-1)}, \quad \widetilde{A}_k \in \mathbb{C}^{(m-k+1)\times(k-1)}$$

where $\widetilde{R}_{k-1}$ is upper triangular and $\widehat{R}_{k-1}$ and $\widetilde{A}_{k-1}$ are dense matrices. The first $k-1$ columns of this transformed A are already upper triangular; we can enforce this condition on column k by working on $\widetilde{A}_{k-1}$.

Let $\widetilde{x}_k \in \mathbb{C}^{m-k+1}$ be the first column of $\widetilde{A}_{k-1}$. We define $\widetilde{Q}_k$ as the $(m-k+1)\times(m-k+1)$ Householder reflector that takes $\widetilde{x}_k$ to $\|\widetilde{x}_k\| e_1 e^{i\theta} \in \mathbb{C}^{m-k+1}$. Then the matrix

$$\widetilde{Q}_k \widetilde{A}_{k-1}$$

has first column proportional to e_1. Therefore, define the unitary transformation $Q_k \in \mathbb{C}^{m\times m}$

$$Q_k = \begin{pmatrix} I_{(k-1)\times(k-1)} & 0 \\ 0 & \widetilde{Q}_k \end{pmatrix}.$$

We have

$$Q_k A = \begin{bmatrix} \widetilde{R}_{k-1} & \widehat{R}_{k-1} \\ 0_{k-1\times n-k+1} & \widetilde{Q}_k \widetilde{A}_{k-1} \end{bmatrix},$$

and therefore this new matrix is upper triangular in its first k columns. We can then proceed by induction, performing a sequence of unitary operations resulting in

$$Q_{q-1} Q_{q-2} \cdots Q_1 A = R,$$

where R is upper triangular and $q = \min(m, n)$. Thus, we have accomplished a QR factorization for A since the product of unitary matrices is unitary.