Department of Mathematics, University of Utah
Analysis of Numerical Methods I
MTH6610 – Section 001 – Fall 2017

Lecture notes: Gram-Schmidt and the QR decomposition

Wednesday September 11, 2019

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

Reading: Trefethen & Bau III, Lecture 7

We have seen that if $\mathcal{V}_k$ is a k-dimensional subspaace of $\mathbb{C}^n$, then there is a unique rank-k matrix P_k that is the orthogonal projector onto $\mathcal{V}_k$. If $q_1, \ldots, q_k$ is any orthonormal basis for this subspace, then

$$P_k = Q_k Q_k^*, \qquad\qquad Q_k = [q_1 \;\; q_2 \;\; \cdots \;\; q_k]$$

This projection matrix is a fundamental tool for orthogonalizing vectors. Note that one can compute $P_k v$ for some $v \in \mathbb{C}^n$ using only inner product operations between q_j and v, and need not explicitly form the matrix P_k.
Let $a_1, \ldots, a_n$ be any basis for $\mathbb{C}^n$. Our goal is to *orthogonalize* these vectors: to arithmetically rearrange them to form an orthonormal basis. The idea is a straightforward: Because the a_j are linearly independent, then a_j is not a linear combination of $a_1, \ldots, a_{j-1}$. Therefore, the following inductive procedure generates an orthonormal set $q_1, \ldots, q_n$ via the scalars r_{ij}:

$$\begin{aligned}
u_1 &= a_1, & r_{11} &= \|u_1\|, & q_1 &= \frac{u_1}{r_{11}} \\
u_2 &= a_2 - P_1 a_2, & r_{22} &= \|u_2\|, & q_2 &= \frac{u_2}{r_{22}} \\
&&& \vdots && \\
u_{k+1} &= a_{k+1} - P_k a_{k+1}, & r_{k+1,k+1} &= \|u_{k+1}\|, & q_{k+1} &= \frac{u_{k+1}}{r_{k+1,k+1}}
\end{aligned}$$

Above, we use $\|\cdot\|$ to mean the vector 2-norm. The $q_1, \ldots, q_n$ are an orthogonalization of the vectors $a_1, \ldots, a_n$. This algorithm is called the *Gram-Schmidt* procedure and can readily be implemented. However, this procedure also reveals a the existence of a particular matrix factoriztion. To see this, we manipulate the expressions above.
Since $P_k a_{k+1}$ lies in the span of $q_1, \ldots, q_k$, then we have

$$P_k a_{k+1} = \sum_{j=1}^{k} r_{j,k+1} q_j, \qquad\qquad r_{j,k+1} = q_j^* a_{k+1}.$$

Then defining the scalars r_{jk} as shown, we have he relations

$$a_{k+1} = u_{k+1} + P_k a_{k+1} = \sum_{j=1}^{k+1} r_{j,k+1} q_j$$

If we identify a_k as columns of a matrix A, then this representation of the vectors a_k is called the QR decomposition of the matrix A. The following result is more general than the procedure we've defined above.

Theorem 1 (QR decomposition/factorization)**.** *Let $A \in \mathbb{C}^{m\times n}$ be a matrix. Then*

$$A = QR, \qquad Q \in C^{m\times m}, \qquad R \in \mathbb{C}^{m\times n}$$

where Q is unitary, and R is an upper triangular matrix. If A is full-rank, the diagonal elements of R can be chosen to be positive.

The columns of A are the vectors a_k, the columns of Q are q_k, and the entries of R are the r_{ij}. If A is not full-rank, then the iterative procedure we've outlined breaks down because one vector u_k will have zero norm. However, this can be remedied by "skipping" the formation of q_k in the orthogonalization procedure.
If $m > n$, then columns $n+1, \ldots, m$ of Q are superfluous and may be omitted. (This is similar in spirit to singular vectors corresponding to zero singular values.) In this case, we may instead have the decomposition $A = \widetilde{Q}\widetilde{R}$, where $\widetilde{Q}$ is $m \times n$ with orthonormal columns, and $\widetilde{R}$ is an $n \times n$ upper triangular matrix. This shorthand version of the full factorization is called the thin/skinny/reduced QR decomposition.