

Mathematical Tripos Part IB: Lent Term 2024

Numerical Analysis – Lecture 15

15 QR factorization (contd)

15.1 Further properties of orthogonal matrices

The Gram-Schmidt algorithm is very unstable: round-off errors accumulate rapidly and, even for moderate values of n , the computed matrix Q is no longer orthogonal. Much better algorithms are based on constructing Q as a composition of certain elementary orthogonal mappings.

Lemma 15.1 A matrix Q is orthogonal $\Leftrightarrow \|Q\mathbf{x}\| = \|\mathbf{x}\| \quad \forall \mathbf{x} \in \mathbb{R}^m$ (i.e., the mapping Q preserves Euclidean length $\|\mathbf{x}\| = \sqrt{(\mathbf{x}, \mathbf{x})}$)

A mapping which preserves the distance between any two points (as orthogonal mapping Q does) is called an *isometry*. It is clear that the composition of two isometrical mappings is an isometry itself. So, the following is true.

Lemma 15.2 If P, Q are orthogonal, so is PQ .

The simplest isometries in $\mathbb{R}^m$ are *rotations* and *reflections*. So, the idea of the next two algorithms is quite clear geometrically: given a sequence of vectors $(\mathbf{a}_i)$ we can always determine a sequence of elementary rotations (reflections) in $\mathbb{R}^m$ that brings the coordinates of $(\mathbf{a}_i)$ to the triangular form.

15.2 Givens rotations

Consider a problem: given $a, b \in \mathbb{R}$, find $c, s \in \mathbb{R}$ such that, with some r ,

$$c^2 + s^2 = 1, \quad \begin{bmatrix} c & s \\ -s & c \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} r \\ 0 \end{bmatrix}.$$

A solution always exists and is given by

$$c = \frac{a}{\sqrt{a^2+b^2}} =: \cos \phi, \quad s = \frac{b}{\sqrt{a^2+b^2}} =: \sin \phi.$$

Generally, for any vector $\mathbf{a}_p \in \mathbb{R}^m$, we can find a matrix $\Omega^{[p,q]}$ such that

$$\Omega^{[p,q]} \mathbf{a}_p = \begin{bmatrix} 1 & & & & \\ & \ddots & & & \\ & & c & s & \\ & & -s & c & \\ & & & & \ddots \\ & & & & & 1 \end{bmatrix} \begin{bmatrix} a_{1p} \\ \vdots \\ a_{pp} \\ \vdots \\ a_{qp} \\ \vdots \\ a_{np} \end{bmatrix} = \begin{bmatrix} a_{1p} \\ \vdots \\ r \\ \vdots \\ 0 \\ \vdots \\ a_{np} \end{bmatrix} \begin{matrix} \leftarrow p \\ \leftarrow q \end{matrix} \quad \begin{aligned} c &= \frac{a_{pp}}{\sqrt{a_{pp}^2 + a_{qp}^2}}, \\ s &= \frac{a_{qp}}{\sqrt{a_{pp}^2 + a_{qp}^2}}. \end{aligned}$$

Such a matrix $\Omega^{[p,q]}$ is called a *Givens rotation*. The mapping $\Omega^{[p,q]}$ rotates the vectors in the two-dimensional plane spanned by $\mathbf{e}_p$ and $\mathbf{e}_q$ (clockwise by the angle ϕ), hence it is orthogonal.

Lemma 15.3 Let A be an $m \times n$ matrix and, for any $1 \leq p \leq q \leq m$, let $\tilde{A} = \Omega^{[p,q]} A$. Then

- 1) $\tilde{a}_{qp} = 0$;
- 2) the p -th and the q -th rows of $\tilde{A}$ are linear combinations of the p -th and q -th rows of A ;
- 3) all other rows of $\tilde{A}$ remains the same as those of A .

Proof. Follows immediately from the form of $\Omega^{[p,q]}$. $\square$

From this lemma it follows that we can subsequently annihilate the subdiagonal elements, column by column, and this implies the next statement.

Theorem 15.4 For any matrix A , there exist Givens matrices $\Omega^{[p,q]}$ such that

$$R := \left(\Omega^{[m-1,m]} \right) \dots \left(\Omega^{[2,m]} \dots \Omega^{[2,3]} \right) \left(\Omega^{[1,m]} \dots \Omega^{[1,3]} \Omega^{[1,2]} \right) A$$

is an upper triangular matrix.

Method 15.5

$$\begin{bmatrix} * & * & * \\ * & * & * \\ * & * & * \\ * & * & * \end{bmatrix} \xrightarrow{\Omega^{[1,2]}} \begin{bmatrix} \bullet & \bullet & \bullet \\ 0 & \bullet & \bullet \\ * & * & * \\ * & * & * \end{bmatrix} \xrightarrow{\Omega^{[1,3]}} \begin{bmatrix} \bullet & \bullet & \bullet \\ 0 & * & * \\ 0 & \bullet & \bullet \\ * & * & * \end{bmatrix} \xrightarrow{\Omega^{[1,4]}} \begin{bmatrix} \bullet & \bullet & \bullet \\ 0 & * & * \\ 0 & * & * \\ 0 & \bullet & \bullet \end{bmatrix} \xrightarrow{\Omega^{[2,3]}} \begin{bmatrix} * & * & * \\ 0 & \bullet & \bullet \\ 0 & 0 & \bullet \\ 0 & * & * \end{bmatrix} \xrightarrow{\Omega^{[2,4]}} \begin{bmatrix} * & * & * \\ 0 & \bullet & \bullet \\ 0 & 0 & * \\ 0 & 0 & \bullet \end{bmatrix} \xrightarrow{\Omega^{[3,4]}} \begin{bmatrix} * & * & * \\ 0 & * & * \\ 0 & 0 & \bullet \\ 0 & 0 & 0 \end{bmatrix}$$

The $\bullet$ -elements have changed through a single rotation while the $*$ -elements remain the same.

The cost. There are less than mn rotations and each rotation replaces two rows by their linear combinations, hence the total cost of computing R is $\mathcal{O}(mn^2)$.

If the matrix Q is required in an explicit form, set $\Omega = I$ and, for each successive rotation, replace Ω by $\Omega^{[p,q]}\Omega$. The final Ω is the product of all the rotations, in correct order, and we let $Q = \Omega^T$. The extra cost is $\mathcal{O}(m^2n)$.

If only one vector $Q^T \mathbf{b}$ is required, we multiply the vector by successive rotations, the cost being $\mathcal{O}(mn)$.

15.3 Householder transformations

Definition 15.6 Given any nonzero $\mathbf{u} \in \mathbb{R}^m$, the $m \times m$ matrix

$$H = H_{\mathbf{u}} = I - \frac{2}{\|\mathbf{u}\|^2} \mathbf{u} \mathbf{u}^T$$

is called a *Householder transformation*, or a *Householder reflection*. Since

$$H\mathbf{u} = -\mathbf{u}, \quad H\mathbf{v} = \mathbf{v} \quad \text{if} \quad \mathbf{u}^T \mathbf{v} = 0,$$

this transformation reflects any vector $\mathbf{x} \in \mathbb{R}^m$ with respect to the $(m-1)$ -dimensional hyperplane orthogonal to $\mathbf{u}$. Each such matrix H is symmetric and (since reflection is an isometry) orthogonal.

Lemma 15.7 For any two vectors $\mathbf{a}, \mathbf{b} \in \mathbb{R}^m$ of equal length, the Householder transformation $H_{\mathbf{u}}$ with $\mathbf{u} = \mathbf{a} - \mathbf{b}$ reflects $\mathbf{a}$ onto $\mathbf{b}$,

$$\mathbf{u} = \mathbf{a} - \mathbf{b}, \quad \|\mathbf{a}\| = \|\mathbf{b}\| \quad \Rightarrow \quad H_{\mathbf{u}} \mathbf{a} = \mathbf{b}.$$

In particular, for any $\mathbf{a} \in \mathbb{R}^m$, the choice $\mathbf{b} = \gamma \mathbf{e}_1$ implies

$$\mathbf{u} = \mathbf{a} - \gamma \mathbf{e}_1, \quad \gamma = \pm \|\mathbf{a}\| \quad \Rightarrow \quad H_{\mathbf{u}} \mathbf{a} = \gamma \mathbf{e}_1.$$

Proof. Draw a picture.

Example 15.8 To reflect

$$\mathbf{a} = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} \xrightarrow{H_{\mathbf{u}}} \begin{bmatrix} \gamma \\ 0 \\ 0 \end{bmatrix} = \gamma \mathbf{e}_1$$

with some $\mathbf{u}$ and γ , we should set $\gamma = \|\mathbf{a}\|$ or $\gamma = -\|\mathbf{a}\|$ to have equal lengths of vectors $\mathbf{a}$ and $\gamma\mathbf{e}_1$, and take

$$\mathbf{u} = \begin{bmatrix} a_1 - \|\mathbf{a}\| \\ a_2 \\ a_3 \end{bmatrix} \quad \text{or} \quad \mathbf{u} = \begin{bmatrix} a_1 + \|\mathbf{a}\| \\ a_2 \\ a_3 \end{bmatrix},$$

respectively. For example, we can reflect

$$\mathbf{a} = \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix} \rightarrow \begin{bmatrix} \gamma \\ 0 \\ 0 \end{bmatrix} = \gamma\mathbf{e}_1$$

either with

$$\gamma = 3 \Rightarrow \mathbf{u} = \begin{bmatrix} -1 \\ 1 \\ 2 \end{bmatrix} \Rightarrow H_{\mathbf{u}}\mathbf{a} = \frac{1}{3} \begin{bmatrix} 2 & 1 & 2 \\ 1 & 2 & -2 \\ 2 & -2 & -1 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix} = \begin{bmatrix} 3 \\ 0 \\ 0 \end{bmatrix},$$

or with

$$\gamma = -3 \Rightarrow \mathbf{u} = \begin{bmatrix} 5 \\ 1 \\ 2 \end{bmatrix} \Rightarrow H_{\mathbf{u}}\mathbf{a} = \frac{1}{15} \begin{bmatrix} -10 & -5 & -10 \\ -5 & 14 & -2 \\ -10 & -2 & 11 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix} = \begin{bmatrix} -3 \\ 0 \\ 0 \end{bmatrix}.$$

Choosing sign of γ . For calculations by hands, it is recommended to choose $\text{sgn } \gamma = \text{sgn } a_1$ as it leads to smaller numbers involved. However, numerically, it is the opposite choice that provides a better stability.

Example 15.9 To reflect

$$\mathbf{a} = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{bmatrix} \xrightarrow{H_{\mathbf{u}}} \begin{bmatrix} a_1 \\ a_2 \\ \gamma \\ 0 \end{bmatrix} = \mathbf{b}$$

we set $\gamma = \pm\sqrt{a_3^2 + a_4^2}$ (to equalize the lengths), and take

$$\mathbf{u} = \mathbf{a} - \mathbf{b} = \begin{bmatrix} 0 \\ 0 \\ a_3 - \gamma \\ a_4 \end{bmatrix}.$$

Theorem 15.10 For any matrix A , there exist Housholder matrices H_k such that

$$R := H_{n-1} \cdots H_2 H_1 A$$

is an upper triangular matrix.

Proof. We take $H_1 = H_{\mathbf{u}}$ with the vector $\mathbf{u} = \mathbf{a} - \gamma\mathbf{e}_1$, and $\mathbf{a}$ being the first column of A . Then $H_1 A$ has $\gamma\mathbf{e}_1$ as its first column. Explicitly,

$$\mathbf{a} = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_m \end{bmatrix} \Rightarrow \mathbf{u} = \begin{bmatrix} a_1 - \gamma \\ a_2 \\ \vdots \\ a_m \end{bmatrix}, \quad \gamma = \pm\|\mathbf{a}\| \Rightarrow H_1 \mathbf{a} = \begin{bmatrix} \gamma \\ 0 \\ \vdots \\ 0 \end{bmatrix}.$$

Suppose that the first $k-1$ columns of $C := H_{k-1} \cdots H_1 A$ have an upper triangular form, and let $\mathbf{c}$ be the k -th column of C . So, we define the next $H_k = H_{\mathbf{u}}$ taking $\mathbf{u}$ by the following rule

$$\mathbf{c} = \begin{bmatrix} c_1 \\ \vdots \\ c_{k-1} \\ c_k \\ c_{k+1} \\ \vdots \\ c_m \end{bmatrix} \Rightarrow \mathbf{u} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ c_k - \gamma \\ c_{k+1} \\ \vdots \\ c_m \end{bmatrix}, \quad \gamma^2 = \sum_{i=k}^m c_i^2 \Rightarrow H_k \mathbf{c} = \begin{bmatrix} c_1 \\ \vdots \\ c_{k-1} \\ \gamma \\ 0 \\ \vdots \\ 0 \end{bmatrix}.$$

The conclusion (that the bottom $m - k$ component of $H_k \mathbf{c}$ will vanish) is due to Lemma 15.7. Also, because of its zero components at the first $k - 1$ positions, such a $\mathbf{u}$ is orthogonal to the previous $k - 1$ columns of C , hence they remain invariant under reflection $H_k C$ (as well as the first $k - 1$ rows of C). Therefore, the first k columns of $H_k C$ have an upper triangular form, and we can proceed further by induction. $\square$

Method 15.11

$$\begin{bmatrix} * & * & * \\ * & * & * \\ * & * & * \\ * & * & * \end{bmatrix} \xrightarrow{H_1} \begin{bmatrix} \bullet & \bullet & \bullet \\ 0 & \bullet & \bullet \\ 0 & \bullet & \bullet \\ 0 & \bullet & \bullet \end{bmatrix} \xrightarrow{H_2} \begin{bmatrix} * & * & * \\ 0 & \bullet & \bullet \\ 0 & 0 & \bullet \\ 0 & 0 & \bullet \end{bmatrix} \xrightarrow{H_3} \begin{bmatrix} * & * & * \\ 0 & * & * \\ 0 & 0 & \bullet \\ 0 & 0 & 0 \end{bmatrix}$$

The $\bullet$ -elements have changed through a single reflection while the $*$ -elements remain the same.

Example 15.12

$$A = \begin{bmatrix} 2 & 4 & 7 \\ 0 & 3 & -1 \\ 0 & 0 & \sqrt{3} \\ 0 & 0 & 4 \end{bmatrix} \Rightarrow \gamma = 5, \quad \mathbf{u} = \begin{bmatrix} 0 \\ 0 \\ -2 \\ 4 \end{bmatrix} \Rightarrow \left(I - 2 \frac{\mathbf{u}\mathbf{u}^T}{\|\mathbf{u}\|^2} \right) A = \begin{bmatrix} 2 & 4 & 7 \\ 0 & 3 & -1 \\ 0 & 0 & \sqrt{5} \\ 0 & 0 & 0 \end{bmatrix}.$$

Calculation of Q and $Q^T \mathbf{b}$. If the matrix Q is required in an explicit form, set $\Omega = I$ initially and, for each successive reflection, replace Ω by $H_u \Omega$. As in the case of Givens rotations, by the end of the computation, $Q = \Omega^T$. The same algorithm is being used to calculate the vector $\mathbf{c} = Q^T \mathbf{b}$.

Remark 15.13 For practical computations notice the following. For a matrix B , respectively a vector $\mathbf{x}$, one should compute the products $H_u B$ and $H_u \mathbf{x}$ as

$$H_u B = B - \frac{2}{\|\mathbf{u}\|^2} \mathbf{u}(\mathbf{u}^T B), \quad H_u \mathbf{x} = \mathbf{x} - 2 \frac{\mathbf{u}^T \mathbf{x}}{\|\mathbf{u}\|^2} \mathbf{u}.$$

Deciding between Givens and Householder transformations. If A is dense, it is in general more convenient to use Householder reflections. Givens rotations come into their own, however, when A has many leading zeros in its rows. In the extreme case, if an $n \times n$ matrix A consists of zeros underneath the first subdiagonal, they can be ‘rotated away’ in just $n - 1$ Givens rotations, at the cost of $\mathcal{O}(n^2)$ operations.