

Mathematical Tripos Part IB: Lent Term 2024

Numerical Analysis – Lecture 14

14 QR factorization

14.1 Inner product spaces

Definition 14.1 An *inner product* on a real vector space $\mathbb{X}$ is a function $(\cdot, \cdot) : \mathbb{X} \times \mathbb{X} \rightarrow \mathbb{R}$ which satisfies the following axioms

- 1) $(x, x) \geq 0 \quad \forall x \in \mathbb{X},$ with equality only if $x = 0$
- 2) $(x, y) = (y, x) \quad \forall x, y \in \mathbb{X},$
- 3) $(\alpha x, y) = \alpha(x, y) \quad \forall \alpha \in \mathbb{R} \quad \forall x, y \in \mathbb{X},$
- 4) $(x + y, z) = (x, z) + (y, z) \quad \forall x, y, z \in \mathbb{X}.$

A vector space with an inner product is called an *inner product space*. If $(x, y) = 0$, then the vectors x, y are called *orthogonal*. A set of vectors $(x_i) \in \mathbb{X}$ is called *orthonormal* if

$$(x_i, x_j) = \delta_{ij} := \begin{cases} 0, & i \neq j; \\ 1, & i = j. \end{cases}$$

For $x \in \mathbb{X}$, the function $\|x\| := (x, x)^{1/2}$ is called the *norm* of x (induced by the given inner product), and we have the Cauchy–Schwarz inequality

$$(x, y) \leq \|x\| \|y\| \quad \forall x, y \in \mathbb{X}.$$

Example 14.2 For $\mathbb{X} = \mathbb{R}^m$, the following rule defines the so-called Euclidean inner product

$$(\mathbf{u}, \mathbf{v}) := \mathbf{u}^T \mathbf{v} := \sum_{i=1}^m u_i v_i, \quad \mathbf{u}, \mathbf{v} \in \mathbb{R}^m.$$

Example 14.3 Another example, which we used in Lecture 3 in construction of orthogonal polynomials, is the inner product on the space $C[a, b]$ of real-valued continuous functions on $[a, b]$ with respect to a fixed positive *weight function* w . It is given by the rule

$$(f, g)_w := \int_a^b [f(x)g(x)] w(x) dx, \quad f, g \in C[a, b].$$

14.2 Orthogonal matrices

Definition 14.4 An $m \times n$ matrix Q ($m \geq n$) is called *orthogonal* if $Q^T Q = I$, e.g., $Q = \frac{1}{3} \begin{bmatrix} 2 & 2 & 1 \\ 1 & -2 & 2 \\ 2 & -1 & -2 \end{bmatrix}$.

Thus, the columns $\mathbf{q}_1, \dots, \mathbf{q}_n \in \mathbb{R}^m$ of the orthogonal Q satisfy $\mathbf{q}_i^T \mathbf{q}_j = \delta_{ij}$, i.e., they are *orthonormal* with respect to the Euclidean inner product in $\mathbb{R}^m$. For a square Q we get

$$Q^{-1} = Q^T, \quad I = Q^T Q = Q Q^T = (Q^T)^T Q^T,$$

therefore, Q^T is also an orthogonal matrix, so that the rows of Q are orthonormal as well. In particular, the column and the row elements of orthogonal $Q \in \mathbb{R}^{n \times n}$ satisfy $\sum_{i=1}^n q_{ij}^2 = \sum_{j=1}^n q_{ij}^2 = 1$. It follows also that a square orthogonal matrix Q is nonsingular. Moreover

$$1 = \det I = \det(Q Q^T) = \det Q \det Q^T = (\det Q)^2 \Rightarrow \det Q = \pm 1.$$

14.3 QR factorization

Definition 14.5 The QR factorization of an $m \times n$ matrix A is the representation

$$A = QR,$$

where Q is an $m \times m$ orthogonal matrix and R is an $m \times n$ upper triangular matrix,

$$\underbrace{\begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & & \vdots \\ a_{n1} & \cdots & a_{nn} \\ \vdots & & \vdots \\ a_{m1} & \cdots & a_{mn} \end{bmatrix}}_n = \underbrace{\begin{bmatrix} q_{11} & \cdots & q_{1n} & \cdots & q_{1m} \\ \vdots & & \vdots & & \vdots \\ q_{n1} & & q_{nn} & & q_{nm} \\ \vdots & & \vdots & & \vdots \\ q_{m1} & \cdots & q_{mn} & \cdots & q_{mm} \end{bmatrix}}_{m \geq n} \underbrace{\begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & & \vdots \\ & & \ddots & \vdots \\ & & & r_{nn} \\ 0 & \cdots & \cdots & 0 \\ \vdots & & & \vdots \\ 0 & \cdots & \cdots & 0 \end{bmatrix}}_n \left. \vphantom{\begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & & \vdots \\ a_{n1} & \cdots & a_{nn} \\ \vdots & & \vdots \\ a_{m1} & \cdots & a_{mn} \end{bmatrix}} \right\} m \geq n.$$

Due to the bottom zero element of R , the columns $q_{n+1}, \dots, q_m$ are inessential for the representation itself, hence we can safely write

$$\begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & & \vdots \\ a_{n1} & \cdots & a_{nn} \\ \vdots & & \vdots \\ a_{m1} & \cdots & a_{mn} \end{bmatrix} = \begin{bmatrix} q_{11} & \cdots & q_{1n} \\ \vdots & & \vdots \\ q_{n1} & \cdots & q_{nn} \\ \vdots & & \vdots \\ q_{m1} & \cdots & q_{mn} \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & & \vdots \\ & & \ddots & \vdots \\ & & & r_{nn} \end{bmatrix}. \quad (14.1)$$

The latter formula is called the *reduced QR factorization*.

Theorem 14.6 Every matrix A has a QR factorization. If A is (square) non-singular, then a factorization $A = QR$ where R has a positive main diagonal is unique.

Proof. Three algorithms of the QR factorization are given below:

- 1) the Gram–Schmidt orthogonalization (for the reduced version),
- 2) the Givens rotations and
- 3) the Householder reflections.

For the second part, let $A = QR$ be non-singular. Then $A^T A = R^T R$ is positive definite, and there is a unique Cholesky factorization $A = \tilde{L} \tilde{L}^T$ with $\tilde{L}$ having a positive main diagonal. Thus, $R = \tilde{L}^T$ is uniquely determined. $\square$

Applications:

- 1) Solution to the linear least squares problem (Lecture 16);
- 2) QR-algorithm for determining eigenvalues (Part II Numerical Analysis).

14.4 The Gram-Schmidt orthogonalization

Let $A = QR$ be sought. If we denote the columns of A and Q by (a_j) and (q_j) respectively, then it follows from (14.1) that, given $(a_k) \in \mathbb{R}^m$, we want to find an orthonormal set $(q_j) \in \mathbb{R}^m$ that satisfies

$$a_k = \sum_{j=1}^k r_{jk} q_j, \quad k = 1 \dots n.$$

The latter problem can be solved for a general inner product space $\mathbb{X}$.

Theorem 14.7 Let $\mathbb{X}$ be an inner product space, and let elements $a_1, \dots, a_n \in \mathbb{X}$ be linearly independent. Then there exist elements $q_1, \dots, q_n \in \mathbb{X}$ such that

$$\sum_{j=1}^k r_{jk} q_j = a_k, \quad k = 1 \dots n, \quad (14.2)$$

$$(q_i, q_j) = \delta_{ij}, \quad i, j = 1 \dots n. \quad (14.3)$$

Proof. From the first equation of (14.2), since $\mathbf{a}_1 \neq 0$,

$$r_{11}\mathbf{q}_1 = \mathbf{a}_1, \quad \|\mathbf{q}_1\| = 1 \Rightarrow r_{11}^2 = (\mathbf{a}_1, \mathbf{a}_1) \Rightarrow r_{11} = \|\mathbf{a}_1\|, \quad \mathbf{q}_1 = \mathbf{a}_1/\|\mathbf{a}_1\|.$$

Suppose that the elements $\mathbf{q}_j$ which satisfy (14.2)-(14.3) are constructed for all $j < k$. The next element $\mathbf{q}_k$ is then constructed as follows (compare with the proof of Lemma 3.1). Firstly, we set

$$\mathbf{b}_k = \mathbf{a}_k - \sum_{j=1}^{k-1} r_{jk}\mathbf{q}_j, \quad r_{jk} = (\mathbf{q}_j, \mathbf{a}_k).$$

From orthonormality of $(\mathbf{q}_j)$, we see that

$$(\mathbf{b}_k, \mathbf{q}_j) = (\mathbf{a}_k, \mathbf{q}_j) - r_{jk} = 0, \quad j < k,$$

i.e. the vector $\mathbf{b}_k$ is orthogonal to all previous $\mathbf{q}_j$. So we just normalize it to get $\mathbf{q}_k$ of the unit length,

$$r_{kk} = \|\mathbf{b}_k\|, \quad \mathbf{q}_k = \mathbf{b}_k/r_{kk}.$$

It follows then that

$$r_{kk}\mathbf{q}_k + \sum_{j=1}^{k-1} r_{jk}\mathbf{q}_j = \mathbf{b}_k + \sum_{j=1}^{k-1} r_{jk}\mathbf{q}_j = \mathbf{a}_k. \quad \square$$

Algorithm 14.8 We may put the previous construction in the following algorithm

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for k = 1 to n do
  b[k] := a[k];
  for j = 1 to k-1 do      #-- void if k=1
    r(j,k) := <q[j], a[k]>;
    b[k] := b[k] - r(j,k)*q[j]
  end
  r(k,k) := sqrt(<b[k], b[k]>);
  q[k] := b[k]/r(k,k)
end

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Example 14.9 QR factorization by Gram-Schmidt of $A = \begin{bmatrix} 2 & 4 & 5 \\ 1 & -1 & 1 \\ 2 & 1 & -1 \end{bmatrix}$.

$$r_{11} = \|\mathbf{a}_1\| = 3, \quad \mathbf{q}_1 = \mathbf{a}_1/r_{11} = \frac{1}{3} \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix};$$

$$r_{12} = (\mathbf{q}_1, \mathbf{a}_2) = 3, \quad \mathbf{b}_2 = \mathbf{a}_2 - r_{12}\mathbf{q}_1 = \begin{bmatrix} 4 \\ -1 \\ 1 \end{bmatrix} - 3 \cdot \frac{1}{3} \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix} = \begin{bmatrix} 2 \\ -2 \\ -1 \end{bmatrix},$$

$$r_{22} = \|\mathbf{b}_2\| = 3, \quad \mathbf{q}_2 = \mathbf{b}_2/r_{22} = \frac{1}{3} \begin{bmatrix} 2 \\ -2 \\ -1 \end{bmatrix};$$

$$r_{13} = (\mathbf{q}_1, \mathbf{a}_3) = 3, \quad r_{23} = (\mathbf{q}_2, \mathbf{a}_3) = 3, \quad \mathbf{b}_3 = \mathbf{a}_3 - r_{13}\mathbf{q}_1 - r_{23}\mathbf{q}_2 = \begin{bmatrix} 5 \\ 1 \\ -1 \end{bmatrix} - 3 \cdot \frac{1}{3} \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix} - 3 \cdot \frac{1}{3} \begin{bmatrix} 2 \\ -2 \\ -1 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ -2 \end{bmatrix},$$

$$r_{33} = \|\mathbf{b}_3\| = 3, \quad \mathbf{q}_3 = \mathbf{b}_3/r_{33} = \frac{1}{3} \begin{bmatrix} 1 \\ 2 \\ -2 \end{bmatrix}.$$

So,

$$A = \begin{bmatrix} 2 & 4 & 5 \\ 1 & -1 & 1 \\ 2 & 1 & -1 \end{bmatrix} = \underbrace{\frac{1}{3} \begin{bmatrix} 2 & 2 & 1 \\ 1 & -2 & 2 \\ 2 & -1 & -2 \end{bmatrix}}_Q \cdot \underbrace{\begin{bmatrix} 3 & 3 & 3 \\ 3 & 3 \\ 3 \end{bmatrix}}_R$$

14.5 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 14.10 *A matrix Q is orthogonal $\Leftrightarrow \|Q\mathbf{x}\| = \|\mathbf{x}\| \ \forall \mathbf{x} \in \mathbb{R}^m$ (i.e., the mapping Q preserves Euclidean norm $\|\mathbf{x}\| = \sqrt{(\mathbf{x}, \mathbf{x})}$)*

Proof. Set $S := Q^T Q$. Then

$$\|Q\mathbf{x}\|^2 = (Q\mathbf{x}, Q\mathbf{x}) = (Q^T Q\mathbf{x}, \mathbf{x}) =: (S\mathbf{x}, \mathbf{x}).$$

If Q is orthogonal, then $S = I$, i.e. $\|Q\mathbf{x}\|^2 = (\mathbf{x}, \mathbf{x}) = \|\mathbf{x}\|^2$. Conversely, if Q is norm-preserving, then

$$(S\mathbf{x}, \mathbf{x}) = (\mathbf{x}, \mathbf{x}) \quad \forall \mathbf{x} \in \mathbb{R}^m \quad (\text{and } S = S^T).$$

Taking $\mathbf{x} = \mathbf{e}_i$, we get $s_{ii} = (S\mathbf{e}_i, \mathbf{e}_i) = 1$, while the choice $\mathbf{x} = \mathbf{e}_i + \mathbf{e}_j$ will provide

$$s_{ii} + s_{ij} + s_{ji} + s_{jj} = 2,$$

whence using $s_{ii} = s_{jj} = 1$ and symmetry of S , we obtain $s_{ij} = s_{ji} = 0$, i.e., $S = I$. $\square$

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 14.11 *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.