MATH50003
Numerical Analysis

III.5 QR Factorisation

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Part III

Numerical Linear Algebra

1. Structured matrices such as banded
2. LU and PLU factorisations for solving linear systems
3. Cholesky factorisation for symmetric positive definite
4. Orthogonal matrices such as Householder reflections
5. QR factorisation for solving least squares

Definition 23 (QR factorisation)**.** The *QR factorisation* is

$$A = QR = \underbrace{\begin{bmatrix} \boldsymbol{q}_1 | \cdots | \boldsymbol{q}_m \end{bmatrix}}_{Q \in U(m)} \underbrace{\begin{bmatrix} \times & \cdots & \times \\ & \ddots & \vdots \\ & & \times \\ & & 0 \\ & & \vdots \\ & & 0 \end{bmatrix}}_{R \in \mathbb{C}^{m \times n}}$$

Definition 24 (Reduced QR factorisation)**.** The *reduced QR factorisation*

$$A = \hat{Q}\hat{R} = \underbrace{\begin{bmatrix} \boldsymbol{q}_1 | \cdots | \boldsymbol{q}_n \end{bmatrix}}_{\hat{Q} \in \mathbb{C}^{m \times n}} \underbrace{\begin{bmatrix} \times & \cdots & \times \\ & \ddots & \vdots \\ & & \times \end{bmatrix}}_{\hat{R} \in \mathbb{C}^{n \times n}}$$

QR gives reduced QR

Embedded in a QR factorisation is the reduced QR

III.5.1 Reduced QR and Gram–Schmidt

Gram–Schmidt is a way of computing the reduced QR

Define
$$\boldsymbol{v}_j := \boldsymbol{a}_j - \sum_{k=1}^{j-1} \underbrace{\boldsymbol{q}_k^\star \boldsymbol{a}_j}_{r_{kj}} \boldsymbol{q}_k$$
$$r_{jj} := \|\boldsymbol{v}_j\|$$
$$\boldsymbol{q}_j := \frac{\boldsymbol{v}_j}{r_{jj}}$$

Theorem (Gram–Schmidt and reduced QR) Define $\boldsymbol{q}_j$ and r_{kj} as above (with $r_{kj} = 0$ if $k > j$). Then a reduced QR factorisation is given by:

$$A = \underbrace{\left[\boldsymbol{q}_1 | \cdots | \boldsymbol{q}_n\right]}_{\hat{Q} \in \mathbb{C}^{m \times n}} \underbrace{\begin{bmatrix} r_{11} & \cdots & r_{1n} \\ & \ddots & \vdots \\ & & r_{nn} \end{bmatrix}}_{\hat{R} \in \mathbb{C}^{n \times n}}$$

III.5.2 Householder reflections and QR

Householder is a more stable way to compute QR

Theorem 7 (QR)**.** *Every matrix $A \in \mathbb{C}^{m\times n}$ has a QR factorisation:*

$$A = QR$$

where $Q \in U(m)$ and $R \in \mathbb{C}^{m\times n}$ is right triangular.

Example 17 (QR by hand). (non examinable)

$$A := \begin{bmatrix} -2 & 0 \\ 2 & 1 \\ 1 & 1 \end{bmatrix} = \underbrace{Q}_{SO(3)} \quad \underbrace{R}_{\mathbb{R}^{3\times 2}}$$

$\vec{a}_1$ (first column)

"right" rectangular

Method 1: Gram – Schmidt (easy by hand), but inaccurate on a computer

Method 2: use Householder. Since $a_{11} < 0$, we want to find

$$Q_1 \quad \text{s.t.} \quad Q_1 \vec{a}_1 = + \|\vec{a}_1\| e_1$$

$$\Rightarrow \quad \|\vec{a}_1\| = \sqrt{4+4+1} = 3 \Rightarrow$$

$$y_1 = \underbrace{\begin{bmatrix}-2\\2\\1\end{bmatrix}}_{\vec{a}_1} \underset{\uparrow \atop \text{סימן } a_{11}}{-} \underbrace{\begin{bmatrix}3\\0\\0\end{bmatrix}}_{\|\vec{a}_1\| e_1} = \begin{bmatrix}-5\\2\\1\end{bmatrix} \Rightarrow \|\vec{y}_1\| = \sqrt{25+4+1}$$

$$= \sqrt{30}$$

$$\Rightarrow \quad \vec{w}_1 = \frac{\vec{y}_1}{\|y_1\|} = \begin{bmatrix}-5\\2\\1\end{bmatrix} \Big/ \sqrt{30} \Rightarrow$$

$$Q_1 = I - 2\,\vec{w}_1^T \vec{w}_1 = \frac{1}{15}\begin{bmatrix}15 & & \\ & 15 & \\ & & 15\end{bmatrix} - \frac{1}{15}\underbrace{\begin{bmatrix}-5\\2\\1\end{bmatrix}\begin{bmatrix}-5 & 2 & 1\end{bmatrix}}_{\begin{bmatrix}25 & -10 & -5\\ -10 & 4 & 2\\ -5 & 2 & 1\end{bmatrix}}$$

III.5.3 QR and least squares

Use QR to solve least squares problems

Theorem 8 (least squares via QR). *Suppose $A \in \mathbb{C}^{m \times n}$ with $m \geq n$ has full rank. Given a QR factorisation $A = QR$ then*

$$\boldsymbol{x} = \hat{R}^{-1}\hat{Q}^\star \boldsymbol{b}$$

minimises $\|A\boldsymbol{x} - \boldsymbol{b}\|$.

$\in \mathbb{C}^n$ $\qquad \in \mathbb{C}^m$

Here $\quad A = \underbrace{QR}_{\text{Full QR}} = \begin{bmatrix} \hat{Q} & K \end{bmatrix} \begin{bmatrix} \hat{R} \\ 0 \end{bmatrix} = \underbrace{\hat{Q}\hat{R}}_{\text{Reduced}}$

Proof $\quad$ We want to minimise $\qquad \tilde{c} := Q^\star \tilde{b}$

$$\|Ax - b\|^2 = \|QRx - b\|^2 = \|Q(R\vec{x} - \overbrace{Q^* \vec{b}})\|^2$$

$$= \|R\vec{x} - \vec{c}\|^2$$

$$= \left\| \underbrace{\begin{bmatrix} x & \cdots & x \\ & \ddots & \vdots \\ & & x \\ & & 0 \\ & & \vdots \\ & & 0 \end{bmatrix}}_{\begin{bmatrix} \hat{R} \\ 0 \end{bmatrix}} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} - \underbrace{\begin{bmatrix} c_1 \\ \vdots \\ c_n \\ \hline c_{n+1} \\ \vdots \\ c_m \end{bmatrix}}_{\begin{bmatrix} \vec{c}_n \\ \vec{k}_n \end{bmatrix}} \right\|^2$$

$$= \|\hat{R}\vec{x} - \vec{c}_n\|^2 + \underbrace{\|\hat{k}_n\|^2}$$

independent of $\tilde{x}$

$\Rightarrow$ $\tilde{x}$ also minimizes

$$\|\hat{R}\,\tilde{x} - \tilde{c}_n\| \Rightarrow$$

$$\tilde{x} = \hat{R}^{-1}\,\tilde{c}_n = \hat{R}^{-1}\,\hat{Q}^{*}\,\tilde{b}$$

since

$$Q^{*}\,\tilde{b} = \begin{bmatrix} \hat{Q}^{*} \\ K^{*} \end{bmatrix} \tilde{b} = \begin{bmatrix} \overbrace{\hat{Q}^{*}\tilde{b}}^{\tilde{c}_n} \\ K^{*}\tilde{b} \end{bmatrix}$$