MA5233 Computational Mathematics

Lecture 4: QR Factorisation

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QR Factorisation

QR factorisation

- An alternative way to solve linear systems.
- A basic building block in many more advanced algorithms.

Outline

- QR factorisation: definition and applications.
- Algorithms:
  - Gram-Schmidt orthogonalisation
  - Householder reflection
  - Givens rotation
- `qr()` in Julia.
- Complexity and stability.

QR Factorisation

QR factorisation

Any $A \in \mathbb{K}^{m \times n}$ can be written as $A = QR$, where

- $Q \in \mathbb{K}^{m \times m}$ is orthogonal ($Q^H Q = I$), and
- $R \in \mathbb{K}^{m \times n}$ is upper triangular ($R(i,j) = 0$ for $i > j$).

Applications

- Solve linear systems (assuming $m = n$):

$$QRx = b \iff x = R^{-1} Q^H b.$$

- Determine orthogonal basis (see next slide).

QR Factorisation

Key property of QR factorisation
Q factor provides an orthogonal basis for range of A.

More precisely:

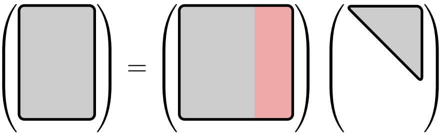
$$
\begin{aligned}
A[:,1] &= Q[:,1]\,R[1,1], \\
A[:,2] &= Q[:,1]\,R[1,2] + Q[:,2]\,R[2,2], \\
A[:,3] &= Q[:,1]\,R[1,3] + Q[:,2]\,R[2,3] + Q[:,3]\,R[3,3] \\
&\dots
\end{aligned}
$$

Conclusion: $\quad \operatorname{span} A[:,1:k] = \operatorname{span} Q[:,1:k].$

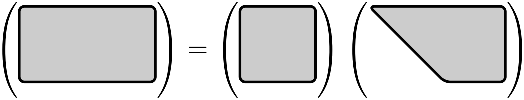
QR Factorisation

Illustration of QR decomposition

Case $m > n$:



Case $m < n$:



Red part of Q factor is redundant since it gets multiplied by zeros in R.
QR factorisation without red part is known as “thin” QR.

QR Factorisation

Algorithms for computing the QR factorisation

- Gram-Schmidt orthogonalisation
- Householder reflections
- Givens rotations

All of these have strengths and weaknesses.
We next go through each of them.

QR Factorisation

Gram-Schmidt theorem
Let $q_1, \ldots, q_k \in \mathbb{K}^n$ be orthonormal and $a_{k+1} \in \mathbb{K}^n$ be linearly independent of the q_k. Then,

$$\tilde{q}_{k+1} := a_{k+1} - \sum_{\ell=1}^{k} q_\ell^H a_{k+1}\, q_\ell$$

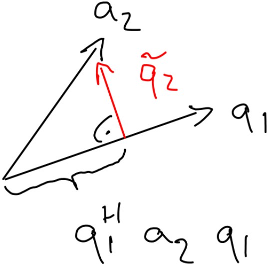
is orthogonal to $q_1, \ldots, q_k$.

Proof.

$$q_\ell^H\, \tilde{q}_{k+1} = q_\ell^H\, a_{k+1} - q_\ell^H q_\ell\, q_\ell^H a_{k+1} = 0.$$

QR Factorisation

Gram-Schmidt theorem, pictorial version



QR Factorisation

QR factorisation via Gram-Schmidt theorem
Rewrite Gram-Schmidt formula

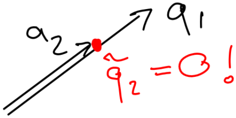
$$\tilde{q}_{k+1} = a_{k+1} - \sum_{\ell=1}^{k} q_\ell^H a_{k+1}\, q_\ell$$

in the form

$$a_{k+1} = \underbrace{\|q_{k+1}\|_2}_{R[k+1,k+1]}\; q_{k+1} + \sum_{\ell=1}^{k} \underbrace{q_\ell^H a_{k+1}}_{R[\ell,k+1]}\, q_\ell .$$

QR Factorisation

Breaking the Gram-Schmidt algorithm



QR Factorisation

Classical Gram-Schmidt

$$\tilde{q}_{k+1}^{(0)} := a_{k+1}, \qquad \tilde{q}_{k+1}^{(\ell+1)} := \tilde{q}_{k+1}^{\ell} - q_\ell^H a_{k+1} \, q_\ell$$

Modified Gram-Schmidt

$$\tilde{q}_{k+1}^{(0)} := a_{k+1}, \qquad \tilde{q}_{k+1}^{(\ell+1)} := \tilde{q}_{k+1}^{(\ell)} - q_\ell^H \tilde{q}_{k+1}^{(\ell)} \, q_\ell$$

Modified Gram-Schmidt is more numerically stable.

QR Factorisation

Example

Classical Gram-Schmidt:

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 0 & \varepsilon & 0 \\ 0 & 0 & \varepsilon \end{pmatrix} \quad \longrightarrow \quad \begin{pmatrix} 1 & \varepsilon_{\mathsf{mach}}\,\varepsilon^{-1} & \varepsilon_{\mathsf{mach}}\,\varepsilon^{-1} \\ 1 & \varepsilon_{\mathsf{mach}}\,\varepsilon^{-1} & \varepsilon_{\mathsf{mach}}\,\varepsilon^{-1} \\ 0 & 1 & \varepsilon_{\mathsf{mach}}\,\varepsilon^{-2} \\ 0 & 0 & 1 \end{pmatrix}$$

Modified Gram-Schmidt:

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 0 & \varepsilon & 0 \\ 0 & 0 & \varepsilon \end{pmatrix} \quad \longrightarrow \quad \begin{pmatrix} 1 & \varepsilon_{\mathsf{mach}}\,\varepsilon^{-1} & \varepsilon_{\mathsf{mach}}\,\varepsilon^{-1} \\ 1 & \varepsilon_{\mathsf{mach}}\,\varepsilon^{-1} & \varepsilon_{\mathsf{mach}}\,\varepsilon^{-1} \\ 0 & 1 & \varepsilon_{\mathsf{mach}}^2\,\varepsilon^{-2} \\ 0 & 0 & 1 \end{pmatrix}$$

QR Factorisation

Householder reflection theorem
Assume $u \in \mathbb{K}^n$ such that $\|u\| = 1$. Then,

$$Q := I - 2\,uu^H$$

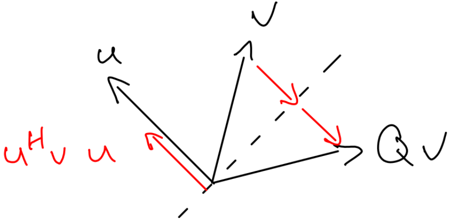
is an orthogonal matrix, and $Q^2 = I$.

Proof.

$$Q^H\,Q = Q^2 = (I - 2\,uu^H)\,(I - 2\,uu^H) = I - 4uu^H + 4u\,(u^H u)\,u^H = I.$$

QR Factorisation

Householder reflection theorem, pictorial version



QR Factorisation

QR factorisation via Householder reflections

Idea: choose u such that $Qa_1 = \pm\alpha e_1$. Then,

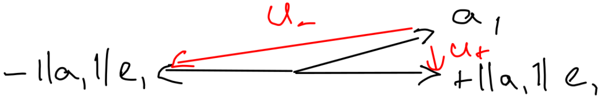
$$Q \begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \end{pmatrix} = \begin{pmatrix} x & x & x \\ 0 & x & x \\ 0 & x & x \end{pmatrix}.$$

How to find $Q = I - 2uu^H$?

QR Factorisation

Determining Householder u

- Reflections preserve length; hence $\alpha = \|a_1\|$.
- $a_1 - u\, u^H a_1 = \pm\|a_1\|\, e_1$ implies $u \propto a_1 \mp \|a_1\|\, e_1$.
- Choose $Qa_1 = -\,\mathrm{sign}(a_{11})\,\|a_1\|\, e_1$ to avoid cancellation in u.
  a_{11} denotes first component of a_1.

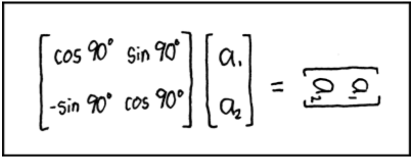


QR Factorisation

Givens rotation

$$Q := \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix} \quad \text{represents a rotation by } \theta.$$

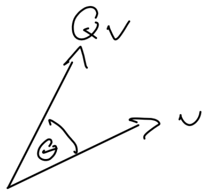
Example



https://xkcd.com/184/

QR Factorisation

Serious example



QR factorisation via Givens rotation

Similar idea as in Householder case:

$$\begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \end{pmatrix} \rightarrow \begin{pmatrix} x & x & x \\ 0 & x & x \\ x & x & x \end{pmatrix} \rightarrow \begin{pmatrix} x & x & x \\ 0 & x & x \\ 0 & x & x \end{pmatrix} \rightarrow \begin{pmatrix} x & x & x \\ 0 & x & x \\ 0 & 0 & x \end{pmatrix}$$

QR Factorisation

QR factorisation in Julia

`F = qr(A)` computes "factorisation object".

- Access factors through `F.Q`, `F.R`, `F.p` (vector) and `F.P` (matrix).
- `F.Q * F.U == A[:,F.p] == A * F.P`.
- `x = F\b` computes solution.

Computational cost of QR factorisation

$\mathcal{O}\big(mn \min\{m,n\}\big)$ floating-point operations.

Stability of Householder QR factorisation

`Q`,`R` computed by Householder QR satisfy

$$\mathtt{Q}\,\mathtt{R} = A + \delta A \qquad \text{where} \qquad \frac{\|\delta A\|}{\|A\|} = \mathcal{O}(\varepsilon_{\mathsf{mach}}).$$

Hence, Householder QR factorisation is backwards stable.

QR Factorisation

References and further reading

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- J. W. Demmel. *Applied Numerical Linear Algebra.* Society for Industrial and Applied Mathematics (1997), `doi:10.1137/1.9781611971446`
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