

AMS526: Numerical Analysis I (Numerical Linear Algebra)

Lecture 12: Stability of Householder QR and Back Substitution

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Outline

1 Stability of Householder QR

2 Stability of Back Substitution

Backward Stability of Householder QR

- For a QR factorization $\mathbf{A} = \mathbf{QR}$ computed by Householder triangularization, the factors $\tilde{\mathbf{Q}}$ and $\tilde{\mathbf{R}}$ satisfy

$$\tilde{\mathbf{Q}}\tilde{\mathbf{R}} = \mathbf{A} + \delta\mathbf{A}, \quad \|\delta\mathbf{A}\|/\|\mathbf{A}\| = O(\epsilon_{\text{machine}}),$$

i.e., exact QR factorization of a slightly perturbed \mathbf{A} (we will not prove it in class)

- $\tilde{\mathbf{R}}$ is \mathbf{R} computed by algorithm using floating points
- However, $\tilde{\mathbf{Q}}$ is product of *exactly unitary* reflectors

$$\tilde{\mathbf{Q}} = \tilde{\mathbf{Q}}_1\tilde{\mathbf{Q}}_2 \dots \tilde{\mathbf{Q}}_n$$

where $\tilde{\mathbf{Q}}_k$ is given by computed $\tilde{\mathbf{v}}_k$, since \mathbf{Q} is not formed explicitly

Backward Stability of Solving $\mathbf{Ax} = \mathbf{b}$ with QR

Algorithm: Solving $\mathbf{Ax} = \mathbf{b}$ by QR Factorization

Compute $\mathbf{A} = \mathbf{QR}$ using Householder, represent \mathbf{Q} by reflectors

Compute vector $\mathbf{y} = \mathbf{Q}^* \mathbf{b}$ implicitly using reflectors

Solve upper-triangular system $\mathbf{Rx} = \mathbf{y}$ for \mathbf{x}

- All three steps are backward stable
- We will prove for backward substitution later
- Overall, we can show that

$$(\mathbf{A} + \Delta\mathbf{A})\mathbf{x} = \mathbf{b}, \quad \|\Delta\mathbf{A}\|/\|\mathbf{A}\| = O(\epsilon_{\text{machine}})$$

as we prove next

Backward Stability of Solving $\mathbf{Ax} = \mathbf{b}$ with Householder QR

Proof: Step 2 gives

$$(\tilde{\mathbf{Q}} + \delta\mathbf{Q})\tilde{\mathbf{y}} = \mathbf{b}, \quad \|\delta\mathbf{Q}\| = O(\epsilon_{\text{machine}})$$

Step 3 gives

$$(\tilde{\mathbf{R}} + \delta\mathbf{R})\tilde{\mathbf{x}} = \tilde{\mathbf{y}}, \quad \|\delta\mathbf{R}\|/\|\mathbf{R}\| = O(\epsilon_{\text{machine}})$$

Therefore,

$$\mathbf{b} = (\tilde{\mathbf{Q}} + \delta\mathbf{Q})(\tilde{\mathbf{R}} + \delta\mathbf{R})\tilde{\mathbf{x}} = \left[\tilde{\mathbf{Q}}\tilde{\mathbf{R}} + (\delta\mathbf{Q})\tilde{\mathbf{R}} + \tilde{\mathbf{Q}}(\delta\mathbf{R}) + (\delta\mathbf{Q})(\delta\mathbf{R}) \right] \tilde{\mathbf{x}}$$

Step 1 gives

$$\mathbf{b} = \left[\mathbf{A} + \underbrace{\delta\mathbf{A} + (\delta\mathbf{Q})\tilde{\mathbf{R}} + \tilde{\mathbf{Q}}(\delta\mathbf{R}) + (\delta\mathbf{Q})(\delta\mathbf{R})}_{\Delta\mathbf{A}} \right] \tilde{\mathbf{x}}$$

where $\tilde{\mathbf{Q}}\tilde{\mathbf{R}} = \mathbf{A} + \delta\mathbf{A}$

Proof of Backward Stability Cont'd

$\tilde{Q}\tilde{R} = \mathbf{A} + \delta\mathbf{A}$ where $\|\delta\mathbf{A}\|/\|\mathbf{A}\| = O(\epsilon_{\text{machine}})$, and therefore

$$\frac{\|\tilde{R}\|}{\|\mathbf{A}\|} \leq \|\tilde{Q}^*\| \frac{\|\mathbf{A} + \delta\mathbf{A}\|}{\|\mathbf{A}\|} = O(1)$$

Now show that each term in $\Delta\mathbf{A}$ is small

$$\frac{\|(\delta\mathbf{Q})\tilde{R}\|}{\|\mathbf{A}\|} \leq \|(\delta\mathbf{Q})\| \frac{\|\tilde{R}\|}{\|\mathbf{A}\|} = O(\epsilon_{\text{machine}})$$

$$\frac{\|\tilde{Q}(\delta\mathbf{R})\|}{\|\mathbf{A}\|} \leq \|\tilde{Q}\| \frac{\|\delta\mathbf{R}\|}{\|\tilde{R}\|} \frac{\|\tilde{R}\|}{\|\mathbf{A}\|} = O(\epsilon_{\text{machine}})$$

$$\frac{\|(\delta\mathbf{Q})(\delta\mathbf{R})\|}{\|\mathbf{A}\|} \leq \|\delta\tilde{Q}\| \frac{\|\delta\mathbf{R}\|}{\|\mathbf{A}\|} = O(\epsilon_{\text{machine}}^2)$$

Overall,

$$\frac{\|\Delta\mathbf{A}\|}{\|\mathbf{A}\|} \leq \frac{\|\delta\mathbf{A}\|}{\|\mathbf{A}\|} + \frac{\|(\delta\mathbf{Q})\tilde{R}\|}{\|\mathbf{A}\|} + \frac{\|\tilde{Q}(\delta\mathbf{R})\|}{\|\mathbf{A}\|} + \frac{\|(\delta\mathbf{Q})(\delta\mathbf{R})\|}{\|\mathbf{A}\|} = O(\epsilon_{\text{machine}})$$

Since the algorithm is backward stable, it is also accurate.

Outline

- 1 Stability of Householder QR
- 2 Stability of Back Substitution

Backward Stability of Back Substitution

- Solve $R\mathbf{x} = \mathbf{b}$ using back substitution

$$\begin{bmatrix} r_{11} & \cdots & r_{1m} \\ & \ddots & \vdots \\ & & r_{mm} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_m \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_m \end{bmatrix}$$

- for $j = m$ downto 1

$$x_j = (b_j - \sum_{k=j+1}^m x_k r_{jk}) / r_{jj}$$

- Back substitute is backward stable

$$(\mathbf{R} + \delta\mathbf{R})\tilde{\mathbf{x}} = \mathbf{b}, \quad \|\delta\mathbf{R}\|/\|\mathbf{R}\| = O(\epsilon_{\text{machine}})$$

Furthermore, each component of $\delta\mathbf{R}$ satisfies

$$\frac{|\delta r_{ij}|}{|r_{ij}|} \leq m\epsilon_{\text{machine}} + O(\epsilon_{\text{machine}}^2)$$

- We will show in full detail for $m = 1, 2, 3$ as well as general m

Proof for B-S of B-S ($m = 1$)

- For $m = 1$, the algorithm is simply one floating point division. Using floating-point axiom, we get

$$\tilde{x}_1 = b_1 \oslash r_{11} = \frac{b_1}{r_{11}}(1 + \epsilon_1) = \frac{b_1}{r_{11}(1 + \epsilon'_1)}$$

where $|\epsilon_1| \leq \epsilon_{\text{machine}}$ and $|\epsilon'_1| \leq \epsilon_{\text{machine}} + O(\epsilon_{\text{machine}}^2)$

- Therefore, we solved a perturbed problem exactly:

$$(r_{11} + \delta r_{11})\tilde{x}_1 = b_1 \quad \text{with} \quad \frac{|\delta r_{11}|}{|r_{11}|} \leq \epsilon_{\text{machine}} + O(\epsilon_{\text{machine}}^2)$$

Proof for B-S of B-S ($m = 2$)

- For $m = 2$, we first solve for \tilde{x}_2 as before. Then, we compute \tilde{x}_1 :

$$\begin{aligned}\tilde{x}_1 &= (b_1 \ominus (\tilde{x}_2 \otimes r_{12})) \oslash r_{11} = \frac{(b_1 - \tilde{x}_2 r_{12}(1 + \epsilon_2))(1 + \epsilon_3)}{r_{11}}(1 + \epsilon_4) \\ &= \frac{b_1 - \tilde{x}_2 r_{12}(1 + \epsilon_2)}{r_{11}(1 + \epsilon'_3)(1 + \epsilon'_4)} = \frac{b_1 - \tilde{x}_2 r_{12}(1 + \epsilon_2)}{r_{11}(1 + 2\epsilon_5)}\end{aligned}$$

where $|\epsilon_2|, |\epsilon_3|, |\epsilon_4| \leq \epsilon_{\text{machine}}$ and
 $|\epsilon'_3|, |\epsilon'_4|, |\epsilon_5| \leq \epsilon_{\text{machine}} + O(\epsilon_{\text{machine}}^2)$

- Again, this is an exact solution to $(R + \delta R)\tilde{x} = b$ with

$$\begin{bmatrix} \frac{|\delta r_{11}|}{|r_{11}|} & \frac{|\delta r_{12}|}{|r_{12}|} \\ & \frac{|\delta r_{22}|}{|r_{22}|} \end{bmatrix} = \begin{bmatrix} 2|\epsilon_5| & |\epsilon_2| \\ & |\epsilon_1| \end{bmatrix} \leq \begin{bmatrix} 2 & 1 \\ & 1 \end{bmatrix} \epsilon_{\text{machine}} + O(\epsilon_{\text{machine}}^2)$$

Proof for B-S of B-S ($m = 3$)

- For $m = 3$, we solve for \tilde{x}_3 and \tilde{x}_2 as before. Then, we compute \tilde{x}_1 :

$$\begin{aligned}\tilde{x}_1 &= [b_1 \ominus (\tilde{x}_2 \otimes r_{12}) \ominus (\tilde{x}_3 \otimes r_{13})] \oslash r_{11} \\ &= \frac{[(b_1 - \tilde{x}_2 r_{12}(1 + \epsilon_4))(1 + \epsilon_6) - \tilde{x}_3 r_{13}(1 + \epsilon_5)](1 + \epsilon_7)}{r_{11}(1 + \epsilon'_8)} \\ &= \frac{b_1 - \tilde{x}_2 r_{12}(1 + \epsilon_4) - \tilde{x}_3 r_{13}(1 + \epsilon_5)(1 + \epsilon'_6)}{r_{11}(1 + \epsilon'_6)(1 + \epsilon'_7)(1 + \epsilon'_8)}\end{aligned}$$

That is, $(\mathbf{R} + \Delta\mathbf{R})\tilde{\mathbf{x}} = \mathbf{b}$ with

$$\begin{bmatrix} \frac{|\delta r_{11}|}{|r_{11}|} & \frac{|\delta r_{12}|}{|r_{12}|} & \frac{|\delta r_{13}|}{|r_{13}|} \\ & \frac{|\delta r_{22}|}{|r_{22}|} & \frac{|\delta r_{23}|}{|r_{23}|} \\ & & \frac{|\delta r_{33}|}{|r_{33}|} \end{bmatrix} \leq \begin{bmatrix} 3 & 1 & 2 \\ & 2 & 1 \\ & & 1 \end{bmatrix} \epsilon_{\text{machine}} + O(\epsilon_{\text{machine}}^2)$$

Proof for B-S of B-S (general m)

- Similar analysis for general m gives pattern

$$\frac{|\delta R|}{|R|} \leq W\epsilon + O(\epsilon_{\text{machine}}^2)$$

where W is (for $m = 5$)

$$\underbrace{\begin{bmatrix} 0 & 1 & 1 & 1 & 1 \\ & 0 & 1 & 1 & 1 \\ & & 0 & 1 & 1 \\ & & & 0 & 1 \\ & & & & 0 \end{bmatrix}}_{\otimes} + \underbrace{\begin{bmatrix} 1 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & 1 & \\ & & & & 1 \end{bmatrix}}_{\ominus} + \underbrace{\begin{bmatrix} 4 & 0 & 1 & 2 & 3 \\ & 3 & 0 & 1 & 2 \\ & & 2 & 0 & 1 \\ & & & 1 & 0 \\ & & & & 0 \end{bmatrix}}_{\ominus}$$

or

$$\begin{bmatrix} 5 & 1 & 2 & 3 & 4 \\ & 4 & 1 & 2 & 3 \\ & & 3 & 1 & 2 \\ & & & 2 & 1 \\ & & & & 1 \end{bmatrix}$$