

Numerical Matrix Analysis

Notes #13 — Conditioning and Stability: Stability of Back Substitution

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Outline

- 1 Looking Back
 - Stability of Householder Triangularization
- 2 Backward Stability of Back Substitution
 - Introduction: Algorithm, Conventions, Axioms, and Theorem
 - Proof
 - Comments

Last Time: Stability of Householder Triangularization

- We discussed the stability properties of QR-factorization by Householder Triangularization (HT-QR).
 - Numerical “evidence” that HT-QR is backward stable.
 - Statement (proof by reference to Higham's *Accuracy and Stability of Numerical Algorithms*) that HT-QR is backward stable

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 - Statement (proof by reference to Higham’s *Accuracy and Stability of Numerical Algorithms*) that HT-QR is backward stable
- Showed that solving $A\vec{x} = \vec{b}$ using HT-QR and backward substitution is backward stable, assuming that
 - (1) $QR = A$ by HT-QR is backward stable
 - (2) $\tilde{w} = Q^* \vec{b}$ is backward stable
 - (3) $R\vec{x} = \tilde{w}$ by back substitution is backward stable

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 - (1) $QR = A$ by HT-QR is backward stable
 - (2) $\tilde{w} = Q^* \vec{b}$ is backward stable
 - (3) $R\vec{x} = \tilde{w}$ by back substitution is backward stable
- **Today:** Explicit proof of (3), and implicit proof of (2).

Backward Stability of Back Substitution

Back substitution is one of the **easiest non-trivial algorithms** we study in numerical linear algebra, and is therefore a good venue for a full backward stability proof.

The proof for backward stability of Householder triangularization follows the same pattern, but the details become more cumbersome.



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Back-substitution applies to $R\vec{x} = \vec{b}$, where

$$\begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1m} \\ & r_{22} & & r_{2m} \\ & & \ddots & \vdots \\ & & & r_{mm} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix}$$

Upper (and lower) triangular matrices are generated by, e.g. the QR-factorization [NOTES#6–7], Gaussian elimination [NOTES#16–17], and the Cholesky factorization [NOTES#17].

Algorithm: Back-Substitution

Algorithm (Back-Substitution)

- 1: $x_m \leftarrow b_m / r_{mm}$
- 2: **for** $\ell \in \{(m-1), \dots, 1\}$ **do**
- 3: $x_\ell \leftarrow \left(b_\ell - \sum_{k=\ell+1}^m x_k r_{\ell k} \right) / r_{\ell\ell}$
- 4: **end for**

Note that the algorithm breaks if $r_{\ell\ell} = 0$ for some ℓ .

For this discussion we make the assumption that $b_\ell - \sum(x_k r_{\ell k})$ is computed as $(m - \ell)$ subtractions performed in k -increasing order.

Simplification: In the theorem/proof, we use the convention that if the denominator in a statement like $\frac{|\delta r_{i\ell}|}{|r_{i\ell}|} \leq m\epsilon_{\text{mach}}$ is zero, we implicitly assert that the numerator is also zero, as $\epsilon_{\text{mach}} \rightarrow 0$. This can be fully formalized, but at this stage it unnecessarily complicates the discussion).

Reference: Key Floating Point Axioms

Floating Point Representation Axiom

$\forall x \in \mathbb{R}$, there exists ϵ with $|\epsilon| \leq \epsilon_{\text{mach}}$,
such that $\text{fl}(x) = x(1 + \epsilon)$.

The Fundamental Axiom of Floating Point Arithmetic

For all $x, y \in \mathbb{F}_n$ (where \mathbb{F}_n is the set of n -bit floating point numbers), there exists ϵ with $|\epsilon| \leq \epsilon_{\text{mach}}$, such that

$$\begin{aligned}x \oplus y &= (x + y)(1 + \epsilon), & x \ominus y &= (x - y)(1 + \epsilon), \\x \otimes y &= (x * y)(1 + \epsilon), & x \oslash y &= (x/y)(1 + \epsilon)\end{aligned}$$

Back-Substitution: Backward Stability Theorem

Theorem (Solving an Upper Triangular System $R\vec{x} = \vec{b}$ Using Back-Substitution is Backward Stable)

Let the back-substitution algorithm be applied to $R\vec{x} = \vec{b}$, where $R \in \mathbb{C}^{m \times m}$ is upper triangular; $\vec{b}, \vec{x} \in \mathbb{C}^m$; in a floating-point environment satisfying the floating point axioms. The algorithm is backward stable in the sense that the computed solution $\tilde{x} \in \mathbb{C}^m$ satisfies

$$(R + \delta R)\tilde{x} = \vec{b}$$

for some upper triangular $\delta R \in \mathbb{C}^{m \times m}$ with

$$\frac{\|\delta R\|}{\|R\|} = \mathcal{O}(\varepsilon_{mach}).$$

Specifically, for each i, ℓ

$$\frac{|\delta r_{i\ell}|}{|r_{i\ell}|} \leq m\varepsilon_{mach} + \mathcal{O}(\varepsilon_{mach}^2).$$



Proof: $m = 1$

When $m = 1$, back substitution terminates in one step

$$\tilde{x}_1 = b_1 \oslash r_{11}$$

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Since we want to express the error in terms of **perturbations of R** , we write

$$\tilde{x}_1 = \frac{b_1}{r_{11}(1 + \epsilon'_1)}, \quad |\epsilon'_1| \leq \varepsilon_{\text{mach}} + \mathcal{O}(\varepsilon_{\text{mach}}^2).$$

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Since we want to express the error in terms of **perturbations of R** , we write

$$\tilde{x}_1 = \frac{b_1}{r_{11}(1 + \epsilon_1')}, \quad |\epsilon_1'| \leq \epsilon_{\text{mach}} + \mathcal{O}(\epsilon_{\text{mach}}^2).$$

Hence,

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

A Note on $(1 + \epsilon)$ and $1/(1 + \epsilon')$

In backward stability proofs we frequently need to move terms of the type $(1 + \epsilon)$ from/to the numerator to/from the denominator.

We do this because we want to express all the floating point errors as perturbations to a specific part of the expression, e.g. the matrix R in the instance of backward substitution.

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When ϵ is small, we can set

$$\epsilon' = \frac{-\epsilon}{1 + \epsilon} \sim -\epsilon(1 - \epsilon + \mathcal{O}(\epsilon^2)) = -\epsilon + \mathcal{O}(\epsilon^2)$$

and thus (**discarding** $\mathcal{O}(\epsilon^2)$ -terms)

$$1 + \epsilon' = \frac{1 + \epsilon}{1 + \epsilon} - \frac{\epsilon}{1 + \epsilon} = \frac{1 + \epsilon - \epsilon}{1 + \epsilon} = \frac{1}{1 + \epsilon} \Rightarrow \frac{1}{1 + \epsilon'} = 1 + \epsilon.$$

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Bottom line: we can move $(1 + \epsilon)$ terms (where $|\epsilon| \leq \epsilon_{\text{mach}} \ll 1$) between the numerator and denominator, and only introduce errors of the order $\mathcal{O}(\epsilon_{\text{mach}}^2)$, i.e. $|\epsilon'| \leq \epsilon_{\text{mach}} + \mathcal{O}(\epsilon_{\text{mach}}^2)$.

Proof: $m = 2$

1 of 2

Step one (which computes \tilde{x}_2) is exactly like the $m = 1$ case:

$$\tilde{x}_2 = \frac{b_2}{r_{22}(1 + \epsilon_1^{\circ})}, \quad |\epsilon_1| \leq \epsilon_{\text{mach}} + \mathcal{O}(\epsilon_{\text{mach}}^2).$$

The second step is defined by

$$\tilde{x}_1 = (b_1 \ominus (\tilde{x}_2 \otimes r_{12})) \oslash r_{11}.$$

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We get

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

Proof: $m = 2$

2 of 2

As before, we can shift the $(1 + \epsilon_3^\ominus)$ and $(1 + \epsilon_4^\ominus)$ terms to the denominator

$$\tilde{x}_1 = \frac{b_1 - \tilde{x}_2 r_{12} (1 + \epsilon_2^\otimes)}{r_{11} (1 + \epsilon_3^{\prime\ominus}) (1 + \epsilon_4^{\prime\ominus})} = \frac{b_1 - \tilde{x}_2 \mathbf{r}_{12} (\mathbf{1} + \epsilon_2^\otimes)}{\mathbf{r}_{11} (\mathbf{1} + \mathbf{2}\epsilon_5^{\ominus, \otimes})}$$

where $|\epsilon'_{3,4}|, |\epsilon_5| \leq \varepsilon_{\text{mach}} + \mathcal{O}(\varepsilon_{\text{mach}}^2)$.

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where $|\epsilon'_{3,4}|, |\epsilon_5| \leq \varepsilon_{\text{mach}} + \mathcal{O}(\varepsilon_{\text{mach}}^2)$.

Now

$$(R + \delta R)\tilde{x} = \vec{b}$$

since \mathbf{r}_{11} is perturbed by the factor $(\mathbf{1} + 2\epsilon_5^{\ominus, \otimes})$, \mathbf{r}_{12} by the factor $(\mathbf{1} + \epsilon_2^\otimes)$, and r_{22} by the factor $(1 + \epsilon_1^\ominus)$.

Proof: $m = 2$

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As before, we can shift the $(1 + \epsilon_3^\ominus)$ and $(1 + \epsilon_4^\ominus)$ terms to the denominator

$$\tilde{x}_1 = \frac{b_1 - \tilde{x}_2 r_{12}(1 + \epsilon_2^\otimes)}{r_{11}(1 + \epsilon_3'^\ominus)(1 + \epsilon_4'^\ominus)} = \frac{b_1 - \tilde{x}_2 \mathbf{r}_{12}(\mathbf{1} + \epsilon_2^\otimes)}{\mathbf{r}_{11}(\mathbf{1} + 2\epsilon_5^{\ominus, \otimes})}$$

where $|\epsilon'_{3,4}|, |\epsilon_5| \leq \varepsilon_{\text{mach}} + \mathcal{O}(\varepsilon_{\text{mach}}^2)$.

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since \mathbf{r}_{11} is perturbed by the factor $(\mathbf{1} + 2\epsilon_5^{\ominus, \otimes})$, \mathbf{r}_{12} by the factor $(\mathbf{1} + \epsilon_2^\otimes)$, and r_{22} by the factor $(1 + \epsilon_1^\ominus)$. The entries satisfy

$$\begin{bmatrix} |\delta r_{11}|/|r_{11}| & |\delta r_{12}|/|r_{12}| \\ & |\delta r_{22}|/|r_{22}| \end{bmatrix} = \begin{bmatrix} 2|\epsilon_5^{\ominus, \otimes}| & |\epsilon_2^\otimes| \\ & |\epsilon_1^\ominus| \end{bmatrix} \leq \begin{bmatrix} 2 & 1 \\ & 1 \end{bmatrix} \varepsilon_{\text{mach}} + \mathcal{O}(\varepsilon_{\text{mach}}^2)$$

Thus $\|\delta R\|/\|R\| = \mathcal{O}(\varepsilon_{\text{mach}})$.

Proof: $m = 3$

1 of 3

The first two steps are as before, and we get

$$\left\{ \begin{array}{l} \tilde{x}_3 = b_3 \oslash r_{33} \\ \tilde{x}_2 = (b_2 \ominus (\tilde{x}_3 \otimes r_{23})) \oslash r_{22} \end{array} \right. = \begin{array}{l} \frac{b_3}{r_{33}(1 + \epsilon_1^\ominus)} \\ \frac{b_2 - \tilde{x}_3 r_{23}(1 + \epsilon_2^\otimes)}{r_{22}(1 + 2\epsilon_3^{\ominus, \ominus})} \end{array}$$

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where superscripts on ϵ s indicate the source operation; now

$$\begin{bmatrix} 2|\epsilon_3| & |\epsilon_2| \\ & |\epsilon_1| \end{bmatrix} \leq \begin{bmatrix} 2 & 1 \\ & 1 \end{bmatrix} \epsilon_{\text{mach}} + \mathcal{O}(\epsilon_{\text{mach}}^2)$$

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We take a deep breath, and write down the third step

$$\tilde{x}_1 = [(b_1 \ominus (\tilde{x}_2 \otimes r_{12})) \ominus (\tilde{x}_3 \otimes r_{13})] \oslash r_{11}$$

Proof: $m = 3$

2 of 3

We expand the two \otimes operations, and write

$$\tilde{x}_1 = [(b_1 \ominus \tilde{x}_2 r_{12}(1 + \epsilon_4^{\otimes})) \ominus \tilde{x}_3 r_{13}(1 + \epsilon_5^{\otimes})] \oslash r_{11}$$

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$$\tilde{x}_1 = [(b_1 \ominus \tilde{x}_2 r_{12}(1 + \epsilon_4^\otimes)) \ominus \tilde{x}_3 r_{13}(1 + \epsilon_5^\otimes)] \oslash r_{11}$$

We introduce error bounds for the \ominus operations

$$\tilde{x}_1 = [(b_1 - \tilde{x}_2 r_{12}(1 + \epsilon_4^\otimes))(1 + \epsilon_6^\ominus) - \tilde{x}_3 r_{13}(1 + \epsilon_5^\otimes)] (1 + \epsilon_7^\ominus) \oslash r_{11}$$

Proof: $m = 3$

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Finally, we convert \oslash to a mathematical division with a perturbation ϵ_8 ; and move both the $(1 + \epsilon_{7,8})$ expressions to the denominator

$$\tilde{x}_1 = \frac{(b_1 - \tilde{x}_2 r_{12}(1 + \epsilon_4^\otimes))(1 + \epsilon_6^\ominus) - \tilde{x}_3 r_{13}(1 + \epsilon_5^\otimes)}{r_{11}(1 + \epsilon_7^\ominus)(1 + \epsilon_8^\oslash)}$$

As it stands, we have introduced a perturbation in b_1 . This was not our intention, so we ship $(1 + \epsilon_6^\ominus)$ to the denominator as well...

Proof: $m = 3$

3 of 3

We now have an expression with perturbations in only $r_{1\ell}$:

$$\tilde{x}_1 = \frac{b_1 - \tilde{x}_2 r_{12}(1 + \epsilon_4^{\otimes}) - \tilde{x}_3 r_{13}(1 + \epsilon_5^{\otimes})(\mathbf{1} + \epsilon_6^{\prime\ominus})}{r_{11}(\mathbf{1} + \epsilon_6^{\prime\ominus})(1 + \epsilon_7^{\prime\ominus})(1 + \epsilon_8^{\prime\ominus})}$$

where $|\epsilon_{4,5}| \leq \varepsilon_{\text{mach}}$, and $|\epsilon'_{6,7,8}| \leq \varepsilon_{\text{mach}} + \mathcal{O}(\varepsilon_{\text{mach}}^2)$.

Proof: $m = 3$

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If we collect the limits on the relative sizes of the perturbations $|\delta r_{i\ell}|/|r_{i\ell}|$ we get the following 6 relations

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

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We are now ready to identify the pattern for general values of $m...$



Proof: General m

1 of 4

The division by r_{ij} induces perturbations δr_{ij} only, since we always immediately shift that $(1 + \epsilon_*)$ -term to the denominator $1/(1 + \epsilon'_*)$, hence the perturbation pattern is of the form

$$\emptyset \rightsquigarrow I_{n \times n} \epsilon_{\text{mach}} + \mathcal{O}(\epsilon_{\text{mach}}^2)$$



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The multiplications $\tilde{x}_i r_{ei}$ induces perturbations δr_{ei} of relative size $\leq \epsilon_{\text{mach}}$, the perturbation pattern is of the form

$$\otimes \rightsquigarrow \begin{bmatrix} 0 & 1 & 1 & \dots & 1 \\ & 0 & 1 & \dots & 1 \\ & & \ddots & \ddots & \vdots \\ & & & 0 & 1 \\ & & & & 0 \end{bmatrix} \epsilon_{\text{mach}}$$

Proof: General m

2 of 4

The most complicated contribution comes from the subtractions (and this is where the order of evaluation has an effect on the answer) — in computing \tilde{x}_k

$r_{k,k}$	is perturbed by	$(1 + \epsilon'_*)^{m-k}$
$r_{k,k+1}$	is perturbed by	0
$r_{k,k+2}$	is perturbed by	$(1 + \epsilon'_*)$
$r_{k,k+3}$	is perturbed by	$(1 + \epsilon'_*)^2$
	\vdots	
$r_{k,m}$	is perturbed by	$(1 + \epsilon'_*)^{m-k-1}$

See next slide for the pattern.

Proof: General m

3 of 4

$$\ominus \rightsquigarrow \begin{bmatrix} (m-1) & 0 & 1 & 2 & 3 & \dots & (m-2) \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ & & 4 & 0 & 1 & 2 & 3 \\ & & & 3 & 0 & 1 & 2 \\ & & & & 2 & 0 & 1 \\ & & & & & 1 & 0 \\ & & & & & & 0 \end{bmatrix} \varepsilon_{\text{mach}} + \mathcal{O}(\varepsilon_{\text{mach}}^2)$$

Putting all this together gives...

Proof: General m — Collecting It All

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$$\frac{|\delta R|}{|R|} \leq \begin{bmatrix} m & 1 & 2 & 3 & 4 & \dots & (m-1) \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ & & 5 & 1 & 2 & 3 & 4 \\ & & & 4 & 1 & 2 & 3 \\ & & & & 3 & 1 & 2 \\ & & & & & 2 & 1 \\ & & & & & & 1 \end{bmatrix} \varepsilon_{\text{mach}} + \mathcal{O}(\varepsilon_{\text{mach}}^2)$$

Which completes the proof. \square

Comments

This is the standard approach for a backward stability analysis.

Errors introduced by the floating point operations \oplus , \ominus , \otimes , and \oslash (in accordance with the axiom) are **reinterpreted** as errors in the initial data / or “problem.”

Where appropriate, errors $\sim \mathcal{O}(\varepsilon_{\text{mach}})$ are freely moved between numerators and denominators.

Perturbations of order $\mathcal{O}(\varepsilon_{\text{mach}})$ are accumulated additively, e.g.

$$(1 + \epsilon_1)(1 + \epsilon_2) = (1 + 2\epsilon_3) + \mathcal{O}(\varepsilon_{\text{mach}}^2)$$

where $|\epsilon_{1,2,3}| \leq \varepsilon_{\text{mach}}$.

Least Squares Problems

Next, we turn our attention back to least squares problems.

- We take a detailed look at the **conditioning** of least squares problems; it is a subtle topic and has nontrivial implications for the **stability** (and ultimately, the **accuracy**) of least squares algorithms.
- Further, this will serve as our main example on detailed conditioning analysis (as Back-substitution served as the main example on detailed backward stability analysis).