Numerical Matrix Analysis

Notes #11 — Conditioning and Stability
Stability... a Closer Look

Peter Blomgren
⟨blomgren@sdsu.edu⟩

Department of Mathematics and Statistics
Dynamical Systems Group
Computational Sciences Research Center
San Diego State University
San Diego, CA 92182-7720

http://terminus.sdsu.edu/

Spring 2024
(Revised: January 18, 2024)

Outline

Student Learning Targets, and Objectives

Target Backward Stability of Basic Floating Point Arithmetic
- **Objective** Know the procedure for showing that $\oplus$, $\ominus$, $\otimes$, and $\oslash$ are backward stable.
- **Objective**

Target ...
- **Objective**
- **Objective**

Last Time: Key Floating Point Axioms

Axiom (Floating Point Representation)

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

Axiom (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 $|\varepsilon| \leq \varepsilon_{\text{mach}}(\mathbb{F}_n)$, such that

$$x \oplus y = (x+y)(1+\varepsilon), \qquad x \ominus y = (x-y)(1+\varepsilon),$$
$$x \otimes y = (x*y)(1+\varepsilon), \qquad x \oslash y = (x/y)(1+\varepsilon)$$

Above, $\texttt{fl} : \mathbb{R} \mapsto \mathbb{F}_n$ is the "function" which takes a real number and produces its n-bit floating point representation.

Last Time: Key Stability Definitions

Definition (Stable Algorithm)

We say that $\tilde{f}$ is a **stable algorithm** if $\forall \vec{x} \in X$

$$\frac{\|\tilde{f}(\vec{x}) - f(\tilde{\vec{x}})\|}{\|f(\tilde{\vec{x}})\|} = \mathcal{O}(\varepsilon_{\text{mach}})$$

for some $\tilde{\vec{x}}$ with

$$\frac{\|\tilde{\vec{x}} - \vec{x}\|}{\|\vec{x}\|} = \mathcal{O}(\varepsilon_{\text{mach}})$$

"A stable algorithm gives approximately the right answer, to approximately the right question."

Last Time: Key Stability Definitions

Definition (Backward Stable Algorithm)

An algorithm $\tilde{f}$ is **backward stable** if $\forall \vec{x} \in X$

$$\tilde{f}(\vec{x}) = f(\tilde{\vec{x}})$$

for some $\tilde{\vec{x}}$ with

$$\frac{\|\tilde{\vec{x}} - \vec{x}\|}{\|\vec{x}\|} = \mathcal{O}(\varepsilon_{\text{mach}})$$

"A backward stable algorithm gives exactly the right answer, to approximately the right question."

Stability: The Road Ahead

- Algorithms: Backward stable, stable, and unstable.
- **Backward Error Analysis** — linking conditioning *(which is a property of the underlying mathematical problem)* and stability *(which is a property of the algorithm)*.
- Detailed Stability Analysis (backward error analysis) of Householder Triangularization.

Floating Point Arithmetic

We start off by showing that our algorithmic building blocks — the floating point operations $\oplus$, $\ominus$, $\otimes$, and $\oslash$ are backward stable.

We look at subtraction, which may be the biggest cause for concern due to cancellation errors. For $\vec{x} = [x_1, x_2]^* \in \mathbb{C}^2$ the **subtraction problem** corresponds to the function

$$f(x_1, x_2) = x_1 - x_2,$$

and the **subtraction algorithm** corresponds to the function

$$\tilde{f}(x_1, x_2) = \texttt{fl}(x_1) \ominus \texttt{fl}(x_2).$$

Floating Point Arithmetic

We apply the floating point representation axiom, and write

$$\texttt{fl}(x_1) = x_1(1+\varepsilon_1), \quad \texttt{fl}(x_2) = x_2(1+\varepsilon_2)$$

for some $|\varepsilon_1|, |\varepsilon_2| \leq \varepsilon_{\text{mach}}$.

By the fundamental axiom of floating point arithmetic, we have

$$\texttt{fl}(x_1) \ominus \texttt{fl}(x_2) = (\texttt{fl}(x_1) - \texttt{fl}(x_2))(1+\varepsilon_3)$$

for some $|\varepsilon_3| \leq \varepsilon_{\text{mach}}$.

Floating Point Arithmetic

Combining these results give us

$$\begin{aligned}\texttt{fl}(x_1) \ominus \texttt{fl}(x_2) &= [x_1(1+\varepsilon_1) - x_2(1+\varepsilon_2)](1+\varepsilon_3)\\ &= x_1(1+\varepsilon_1)(1+\varepsilon_3) - x_2(1+\varepsilon_2)(1+\varepsilon_3)\\ &= \underbrace{x_1(1+\varepsilon_4)}_{\tilde{x}_1} - \underbrace{x_2(1+\varepsilon_5)}_{\tilde{x}_2},\end{aligned}$$

for some $|\varepsilon_4|, |\varepsilon_5| \leq 2\varepsilon_{\text{mach}} + \mathcal{O}(\varepsilon_{\text{mach}}^2)$.

Hence $\tilde{f}(x_1, x_2) = \tilde{x}_1 - \tilde{x}_2 \equiv f(\tilde{x}_1, \tilde{x}_2)$, where

$$\frac{|\tilde{x}_1 - x_1|}{|x_1|} = \mathcal{O}(\varepsilon_{\text{mach}}), \qquad \frac{|\tilde{x}_2 - x_2|}{|x_2|} = \mathcal{O}(\varepsilon_{\text{mach}}).$$

Hence **floating point subtraction is a backward stable operation.**

Floating Point Arithmetic

We have shown that **floating point subtraction is a backward stable operation.**

However, from [LECTURE#9] we know that **subtraction is potentially ill-conditioned:**

$$\kappa(\vec{x}) = \frac{\|J(\vec{x})\|_\infty}{\|f(\vec{x})\|/\|\vec{x}\|_\infty} = \frac{2\,\max\{|x_1|, |x_2|\}}{|x_1 - x_2|}.$$

These are NOT contradictory statements!

Example: Inner Product $\vec{x}^*\vec{y}$

Given two vectors $\vec{x}, \vec{y} \in \mathbb{C}^m$, the computed value of the inner product

$$\alpha = \vec{x}^*\vec{y} = \sum_{i=1}^{m} x_i^* y_i$$

is (usually) given by

$$\tilde{\alpha} = (\texttt{fl}(x_1^*)\otimes\texttt{fl}(y_1))\oplus(\texttt{fl}(x_2^*)\otimes\texttt{fl}(y_2))\oplus\cdots\oplus(\texttt{fl}(x_m^*)\otimes\texttt{fl}(y_m)).$$

Built from the backward stable fundamental operations in this manner, **the inner product is also backward stable.** (We leave the proof of this for later).

Example: Outer Product $\vec{x}\vec{y}^*$

Given $\vec{x} \in \mathbb{C}^m$, and $\vec{y} \in \mathbb{C}^n$, the $A \in \mathbb{C}^{m \times n}$ rank-1 outer product is given by

$$A = \vec{x}\vec{y}^* = \begin{bmatrix} x_1\vec{y}^* \\ x_2\vec{y}^* \\ \vdots \\ x_m\vec{y}^* \end{bmatrix}$$

The obvious algorithm is to compute the mn products $x_i y_j^*$ with $\otimes$ and collect the results into the matrix $\tilde{A}$.

This algorithm is **stable, but not backward stable**. — The matrix $\tilde{A}$ will most likely not have rank 1, and can therefore not be written in the form $(\vec{x} + \delta\vec{x})(\vec{y} + \delta\vec{y})^*$.

Example: $(x + \mathcal{C})$

Let $\mathcal{C} \in \mathbb{C}$ be a fixed non-zero constant, and consider computing $(x + \mathcal{C})$, given $x \in \mathbb{C}$, we get

$$\begin{aligned} \tilde{f}(x) &= \mathtt{fl}(x) \oplus \mathtt{fl}(\mathcal{C}) \\ &= (x(1+\varepsilon_1) + \mathcal{C}(1+\varepsilon_2))\,(1+\varepsilon_3) \\ &= x(1+\varepsilon_4) + \mathcal{C}(1+\varepsilon_5), \end{aligned}$$

with $|\varepsilon_1|, |\varepsilon_2|, |\varepsilon_3| \le \varepsilon_{\text{mach}}$, $|\varepsilon_4|, |\varepsilon_5| \le 2\varepsilon_{\text{mach}} + \mathcal{O}(\varepsilon_{\text{mach}}^2)$.

When $\mathcal{C} \ne 0$, and $x \approx 0$ we are introducing errors of size $\mathcal{O}(\varepsilon_{\text{mach}})$, independent of x. Relative to the size of x, these errors may become unbounded.

Therefore, we cannot interpret the errors as being caused by small perturbations in the data. Hence $(x + \mathcal{C})$ **is not backward stable.**

Notes

Rule of Thumb:

As a rule, algorithms $\tilde{F} : X \mapsto Y$, where the dimension of Y is greater than the dimension of X are rarely backward stable.
In the outer product example, X has dimension $(m+n)$, and Y has dimension $(m \cdot n)$.

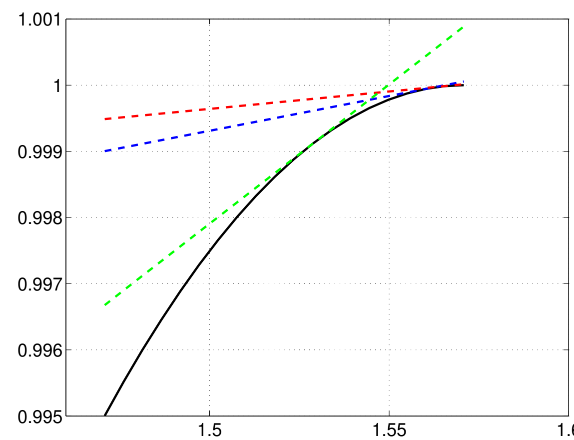
Confusing?

Note that $\tilde{f}(x) = (x + \mathcal{C})$ is not backward stable for fixed $\mathcal{C} \ne 0$, but the algorithm for $\tilde{f}(x, y) = (x + y)$ is backward stable.

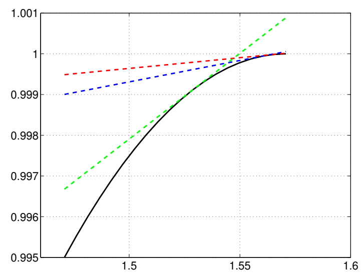
Example: $\sin(x)$ and $\cos(x)$

Floating point calculations of $\sin(x)$ and $\cos(x)$ are stable, but not backward stable.

Consider $\sin(x)$ for $x = \left(\frac{\pi}{2} - \delta\right)$, $0 < \delta \ll 1$,



Example: sin(x) and cos(x)



Suppose we have computed $\tilde{f}(x) = \texttt{fl}(\sin(x)) = \sin(x)(1+\varepsilon_1)$.
Since $f'(x) = \cos(x) \approx \delta$, we have [Remember Taylor, $\delta f = f'(x)\,\delta x$]

$$\tilde{f}(x) = f(\tilde{x}) \text{ for some } \tilde{x} \text{ with } (\tilde{x} - x) \approx \frac{1}{\delta}(\tilde{f}(x) - f(x)) = \mathcal{O}\left(\frac{\varepsilon_{\text{mach}}}{\delta}\right).$$

Since δ can be arbitrarily small, the backward error is not of magnitude $\mathcal{O}(\varepsilon_{\text{mach}})$.
We have an "exact solution", but not to a "nearby problem."

Example: Eigenvalues of a Matrix

One way of computing the eigenvalues of a square matrix, $A \in \mathbb{R}^{m \times m}$, is through the use of the **characteristic polynomial**

$$p(\lambda) = \det(\lambda I - A).$$

The m roots $\{\lambda_1, \lambda_2, \ldots, \lambda_m\}$, where $p(\lambda_i) = 0$ are the eigenvalues of A. Hence, the following algorithm seems reasonable at first glance:

1. Find the coefficients of the characteristic polynomial.
2. Find its roots.

Unfortunately, this algorithm is not only not backward stable, but also unstable; and performs especially badly when the polynomial is expressed in the monomial standard basis $\{\, x^k \,\}_{k=0,1,\ldots,m}$.

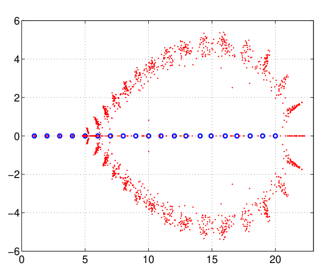
Even when the eigenvalue problem is well-conditioned, this algorithm may produce answers with large relative errors.

Example: Eigenvalues of a Matrix

The instability manifests itself in the root-finding step. Recall Wilkinson's example [LECTURE#9], where relative perturbations of the coefficients of

$$p_{\text{Wilkinson}}(x) = \prod_{i=1}^{20}(x - i) = a_0 + a_1 x + \cdots + a_{19}x^{19} + x^{20}$$

by $\sim 10^{-10}$ resulted in perturbation of size $\sim$ 1–10 of the roots



Example: Eigenvalues of a Matrix

The characteristic polynomial of the diagonal matrix

$$A_1 = \text{diag}(1, 2, \ldots, 20)$$

is a Wilkinson polynomial or degree 20.

An even simpler example is given by $A_2 = \text{diag}(1, 1)$, the (2×2)-identity. Trying to find the roots of the characteristic polynomial $p_2(\lambda) = \lambda^2 - 2\lambda + 1$, reminds us of the example (also in [LECTURE#9]) leading up to Wilkinson's polynomial:

$$\begin{aligned} x^2 - 2x + 1 &= (x-1)^2 \\ x^2 - 2x + 0.9999 &= (x - 0.99)(x - 1.01) \\ x^2 - 2x + 0.999999 &= (x - 0.999)(x - 1.001). \end{aligned}$$

Where the algorithm above produces errors $\mathcal{O}(\sqrt{\varepsilon_{\text{mach}}})$.

Example: Eigenvalues of a Matrix

But really... This is a little too pessimistic. IEEE-785-1985 floating point $\mathbb{F}_{64}$ can represent ("small$^{\times}$") integers exactly... But if we try

$$A = \begin{bmatrix} 1+10^{-14} & 0 \\ 0 & 1 \end{bmatrix}$$

with $p(\lambda) = \lambda^2 - (2+10^{-14})\lambda + (1+10^{-14})$, then in an environment where $\varepsilon_{\text{mach}} = 2.22 \times 10^{-16}$ we get

$$\{\tilde{\lambda}_1, \tilde{\lambda}_2\} = \{0.99999998509884, 1.00000001490117\}$$

with errors

$$\{\tilde{\lambda}_1 - 1, \tilde{\lambda}_2 - (1+10^{-14})\} = \{-1.49 \times 10^{-8}, 1.49 \times 10^{-8}\} \sim \mathcal{O}(\sqrt{\varepsilon_{\text{mach}}})$$

$^{\times}$ Definition of small in $\mathbb{F}_{64}$: $|n| \leq 9,007,199,254,740,992$.

Accuracy of a Backward Stable Algorithm

Suppose we have a backward stable algorithm $\tilde{f}$ for the problem $f : X \mapsto Y$.

The Real Question: Will the results be accurate?

Answer: It depends... on the condition number $\kappa = \kappa(x)$.

If $\kappa(x)$ is small, the results will be accurate. When $\kappa(x)$ is large, the results may be unreliable.

We always lose accuracy in proportion to the size of $\kappa(x)$.

We make this dependence precise in a theorem...

Accuracy of a Backward Stable Algorithm

Theorem (Computational Accuracy)

Suppose a backward stable algorithm $\tilde{f}$ is applied to solve a problem $f : X \mapsto Y$ with condition number $\kappa(x)$ in a floating point environment satisfying the floating point representation axiom, and the fundamental axiom of floating point arithmetic.

Then the relative errors satisfy

$$\frac{\|\tilde{f}(x) - f(x)\|}{\|f(x)\|} = \mathcal{O}(\kappa(x)\varepsilon_{mach})$$

We have tied conditioning, stability, and accuracy together!

Accuracy of a Backward Stable Algorithm

Proof (Computational Accuracy)

By the definition of backward stability, we have $\tilde{f}(x) = f(\tilde{x})$ for some $\tilde{x} \in X$, with

$$\frac{\|\tilde{x} - x\|}{\|x\|} = \mathcal{O}(\varepsilon_{\text{mach}}).$$

By the definition of $\kappa(x)$

$$\kappa(x) = \sup_{\delta x} \left[\frac{\|\delta f\|}{\|f(x)\|} \Big/ \frac{\|\delta x\|}{\|x\|} \right],$$

we have

$$\frac{\|\tilde{f}(x) - f(x)\|}{\|f(x)\|} \leq (\kappa(x) + o(1)) \frac{\|\tilde{x} - x\|}{\|x\|} = \mathcal{O}(\kappa(x)\varepsilon_{\text{mach}}). \quad \square$$

Note: $o(1)$ is a quantity which converges to zero as $\varepsilon_{\text{mach}} \to 0$.

Backward Error Analysis

The method of proof we used defines the strategy for **backward error analysis**.

We obtain the accuracy estimate in two steps:

1. Analyze the **condition** of the problem.
2. Analyze the **stability** of the algorithm.

Conclusion: **If the algorithm is backward stable, then the accuracy is proportional to the condition number.**

At this point, this may seem natural and straight-forward?

Naively, *Forward Error Analysis* may seem like a tempting alternative...

Forward Error Analysis... ...and Backward Error Analysis

At first glance, the most natural form of error analysis is to apply the *the floating point representation axiom*, and *the fundamental axiom of floating point arithmetic* directly to the algorithms and

1. Introduce error bounds on each operations.
2. Track how the errors compound throughout the computation.

It turns out that this approach is very difficult to carry out successfully.

Here there is no separation of algorithm and problem; hence the forward error analysis must capture both the stability behavior of the algorithm, **and** the conditioning of the problem. How do we "detect" the conditioning in operation-level analysis?!?

Backward Error Analysis

Backward Error Analysis is the right tool: in general, the **best** algorithms for a problem will compute the exact solution to a slightly perturbed problem. The method of backward error analysis is perfectly tailored to this slightly "backward view."

Next Time ...and The Near Future

We carefully analyze the stability of two of our most important algorithms:

- The Householder Triangularization algorithm for computing the QR-factorization.
- The back (and forward) substitution algorithm.

Together they are the foundation upon with we build our solvers for $A\vec{x} = \vec{b}$ for both square and non-square A.

Then, we re-visit the Least Squares problem — and carefully look at the conditioning of the problem, and stability of the algorithms we use for solving the problem.