Numerical Matrix Analysis

Notes #10 — Conditioning and Stability
Floating Point Arithmetic / Stability

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 Floating Point Arithmetic

- Objective Know how to express a floating point unmber using the IEEE-785-1985 (and successor) standard
- Objective Know how to express the limits of the floating point environment using $\varepsilon_{\text{mach}}$.

Target Stability

- Objective Know the definitions of absolute and relative error.
- Objective Know the formal and informal definitions of stable and backward stable algorithms.

Finite Precision — A 64-bit real number, `double`

The **Binary Floating Point Arithmetic Standard** 754-1985 (IEEE — The Institute for Electrical and Electronics Engineers) standard specified the following layout for a 64-bit real number:

$$\mathbf{s\, c_{10}\, c_9\, \ldots\, c_1\, c_0\, m_{51}\, m_{50}\, \ldots\, m_1\, m_0}$$

Where

Symbol	Bits	Description
s	1	The sign bit — 0=positive, 1=negative
c	11	The characteristic (exponent)
m	52	The mantissa

$$r = (-1)^s\, 2^{c-1023}\,(1+f), \qquad c = \sum_{n=0}^{10} c_n 2^n, \qquad f = \sum_{k=0}^{51} \frac{m_k}{2^{52-k}}$$

IEEE-754-1985 Special Signals

In order to be able to represent **zero**, ±∞, and **NaN** (not-a-number), the following special signals are defined in the IEEE-754-1985 standard:

Type	S (1 bit)	C (11 bits)	M (52 bits)
signaling NaN	u	2047 (max)	.0uuuuu—u (*)
quiet NaN	u	2047 (max)	.1uuuuu—u
negative infinity	1	2047 (max)	.000000—0
positive infinity	0	2047 (max)	.000000—0
negative zero	1	0	.000000—0
positive zero	0	0	.000000—0

(*) with at least one 1 bit.

From `http://www.freesoft.org/CIE/RFC/1832/32.htm`

If you think IEEE-754-1985 is too "simple." There are some interesting additions in the IEEE 754-2008 revision; *e.g.* fused-multiply-add (`fma`) operations.

Some environments (e.g. AVX/AVX2/AVX-512 extensions) combine multiple `fma` operations into a single step, e.g. performing a four-element dot-product on two 128-bit SIMD registers $a_0 \times b_0 + a_1 \times b_1 + a_2 \times b_2 + a_3 \times b_3$ with single cycle throughput.

Examples: Finite Precision

$$r = (-1)^s\, 2^{c-1023}\,(1+f), \quad c = \sum_{k=0}^{10} c_n 2^n, \quad f = \sum_{k=0}^{51} \frac{m_k}{2^{52-k}}$$

Example #1 — 3.0

$$0, 10000000000, 1000000000000000000000000000000000000000000000000000$$

$$r_1 = (-1)^0 \cdot 2^{2^{10}-1023} \cdot \left(1 + \frac{1}{2}\right) = 1 \cdot 2^1 \cdot \frac{3}{2} = 3.0$$

Example #2 — (The Smallest Positive Real Number)

$$0, 00000000000, 0000000000000000000000000000000000000000000000000001$$

$$r_2 = (-1)^0 \cdot 2^{0-1023} \cdot (1 + 2^{-52}) \approx 1.113 \times 10^{-308}$$

Examples: Finite Precision

$$r = (-1)^s\, 2^{c-1023}\,(1+f), \quad c = \sum_{k=0}^{10} c_n 2^n, \quad f = \sum_{k=0}^{51} \frac{m_k}{2^{52-k}}$$

Example #3 — (The Largest Positive Real Number)

$$0, 11111111110, 1111111111111111111111111111111111111111111111111111$$

$$\begin{aligned} r_3 &= (-1)^0 \cdot 2^{1023} \cdot \left(1 + \frac{1}{2} + \frac{1}{2^2} + \cdots + \frac{1}{2^{51}} + \frac{1}{2^{52}}\right) \\ &= 2^{1023} \cdot \left(2 - \frac{1}{2^{52}}\right) \approx 1.798 \times 10^{308} \end{aligned}$$

That's Quite a Range!

In summary, we can represent

$$\left\{ \pm 0, \quad \pm 1.113 \times 10^{-308}, \quad \pm 1.798 \times 10^{308}, \quad \pm\infty, \quad \texttt{NaN} \right\}$$

and a whole bunch of numbers in

$$(-1.798 \times 10^{308},\ -1.113 \times 10^{-308}) \cup (1.113 \times 10^{-308},\ 1.798 \times 10^{308})$$

Bottom line: Over- or under-flowing is usually not a problem in IEEE floating point arithmetic.

The problem in **scientific computing** is what we **cannot** represent.

Fun with Matlab... ...Integers

$$\begin{array}{rcrcl}
(2^{53}+2) & - & 2^{53} & = & 2 \\
(2^{53}+2) & - & (2^{53}+1) & = & 2 \\
(2^{53}+1) & - & 2^{53} & = & 0 \\
2^{53} & - & (2^{53}-1) & = & 1
\end{array}$$

$$\texttt{realmax} = 1.7977 \cdot 10^{308} \qquad \texttt{realmin} = 2.2251 \cdot 10^{-308}$$
$$\texttt{eps} = 2.2204 \cdot 10^{-16}$$

The smallest not-exactly-representable integer is $(2^{53}+1) = 9,007,199,254,740,993.$

Something is Missing — Gaps in the Representation 1 of 3

There are gaps in the floating-point representation!

Given the representation

0 00000000000 0000000000000000000000000000000000000000000000000001

for the value $v_1 = 2^{-1023}(1 + 2^{-52})$,

the next larger floating-point value is

0 00000000000 0000000000000000000000000000000000000000000000000010

i.e. the value $v_2 = 2^{-1023}(1 + 2^{-51})$

The difference between these two values is $2^{-1023} \cdot 2^{-52} = 2^{-1075}$ $(\sim 10^{-324})$.

Any number in the interval (v_1, v_2) **is not representable!**

Something is Missing — Gaps in the Representation 2 of 3

A gap of 2^{-1075} doesn't seem too bad...

However, the size of the gap depend on the value itself...

Consider $r = 3.0$

0 10000000000 1000000000000000000000000000000000000000000000000000

and the next value

0 10000000000 1000000000000000000000000000000000000000000000000001

Here, the difference is $2 \cdot 2^{-52} = 2^{-51}$ $(\sim 10^{-16})$.

In general, in the interval $[2^n, 2^{n+1}]$ the gap is 2^{n-52}.

Something is Missing — Gaps in the Representation 3 of 3

At the other extreme, the difference between

0 11111111110 1111111111111111111111111111111111111111111111111110

and the next value

0 11111111110 1111111111111111111111111111111111111111111111111111

is $2^{1023} \cdot 2^{-52} = 2^{971} \approx 1.996 \cdot 10^{292}$.

That's a fairly significant gap!!! (A number large enough to comfortably count all the particles in the universe...)

See, *e.g.*

https://physics.stackexchange.com/ ...

questions/47941/dumbed-down-explanation-how-scientists-know-the-number-of-atoms-in-the-universe

The Relative Gap

It makes more sense to factor the exponent out of the discussion and talk about the relative gap:

Exponent	**Gap**	**Relative Gap (Gap/Exponent)**
2^{-1023}	2^{-1075}	$2^{-52} \approx 2.22 \times 10^{-16}$
2^{1}	2^{-51}	2^{-52}
2^{1023}	2^{971}	2^{-52}

Any difference between numbers smaller than the local gap is not representable, *e.g.* any number in the interval

$$\left[3.0,\ 3.0 + \frac{1}{2^{51}}\right)$$

is represented by the value 3.0.

The Floating Point "Theorem"

$\varepsilon_{\text{mach}}$

"Theorem"

Floating point "numbers" represent intervals!

Notation

We let $\texttt{fl}(x)$ denote the floating point representation of $x \in \mathbb{R}$.

Let the symbols $\oplus$, $\ominus$, $\otimes$, and $\oslash$ denote the floating-point operations: addition, subtraction, multiplication, and division.

The Floating Point $\varepsilon_{\text{mach}}$

The relative gap defines $\varepsilon_{\text{mach}}$; and

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

In 64-bit floating point arithmetic $\varepsilon_{\text{mach}} \approx 2.22 \times 10^{-16}$.

In matlab, `eps` returns this value.

In Python, `print(np.finfo(float).eps)`

In C, `#include <float.h>` to define the value of `__DBL_EPSILON__`

Floating Point Arithmetic

$\varepsilon_{\text{mach}}$

All floating-point operations are performed up to some precision, *i.e.*

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

This paired with our definition of $\varepsilon_{\text{mach}}$ gives us

Axiom (The Fundamental Axiom of Floating Point Arithmetic)

For an n-bit floating point environment —
For all $x, y \in \mathbb{F}_{64}$ (where $\mathbb{F}_{64}$ is the set of 64-bit floating point numbers), there exists ε with $|\varepsilon| \le \varepsilon_{\text{mach}}(\mathbb{F}_{64})$, such that

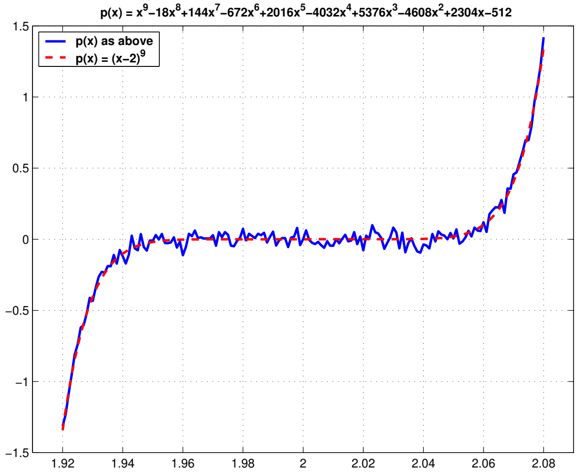
$$\begin{aligned} x \oplus y &= (x+y)(1+\varepsilon), & x \ominus y &= (x-y)(1+\varepsilon), \\ x \otimes y &= (x*y)(1+\varepsilon), & x \oslash y &= (x/y)(1+\varepsilon) \end{aligned}$$

That is **every operation of floating point arithmetic is exact up to a relative error of size at most $\varepsilon_{\text{mach}}$**.

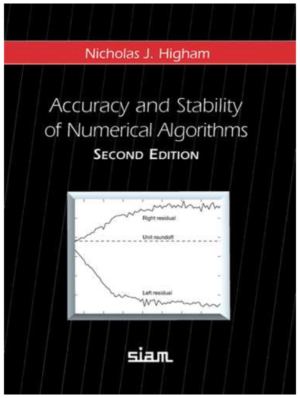
Example: Floating Point Error Scaled by 10^{10}

Consider the following polynomial on the interval [1.92, 2.08]:

$$\begin{aligned} p(x) &= (x-2)^9 \\ &= x^9 - 18x^8 + 144x^7 - 672x^6 + 2016x^5 - 4032x^4 + 5376x^3 - 4608x^2 + 2304x - 512 \end{aligned}$$



Stability



Nicholas J. Higham
Accuracy and Stability of Numerical Algorithms
Second Edition
siam

680 pages of details...

Stability: Introduction 1 of 3

With the knowledge that **"(floating point) errors happen,"** we have to re-define the concept of the **"right answer."**

Previously, in the context of **conditioning** we defined a mathematical problem as a map

$$f : X \mapsto Y$$

where $X \subseteq \mathbb{C}^n$ is the set of data (input), and $Y \subseteq \mathbb{C}^m$ is the set of solutions.

Stability: Introduction 2 of 3

We now define an implementation of an **algorithm** — on a floating-point device, where $\mathbb{F}$ satisfies the fundamental axiom of floating point arithmetic — as another map

$$\tilde{f} : X \mapsto Y$$

i.e. $\tilde{f}(\vec{x}) \in Y$ is a numerical solution of the problem.

Wiki-History: Pentium FDIV bug (≈ 1994)

The Pentium FDIV bug was a bug in Intel's original Pentium FPU. Certain FP division operations performed with these processors would produce incorrect results. According to Intel, there were a few missing entries in the lookup table used by the divide operation algorithm.

Although encountering the flaw was extremely rare in practice (*Byte Magazine* estimated that 1 in 9 billion FP divides with random parameters would produce inaccurate results), both the flaw and Intel's initial handling of the matter were heavily criticized. Intel ultimately recalled the defective processors.

Stability: Introduction 3 of 3

The task at hand is to make **useful** statements about $\tilde{f}(\vec{x})$.

Even though $\tilde{f}(\vec{x})$ is affected by many factors — roundoff errors, convergence tolerances, competing processes on the computer*, etc; we will be able to make (maybe surprisingly) clear statements about $\tilde{f}(\vec{x})$.

* Note that depending on the memory model, the previous state of a memory location *may* affect the result in *e.g.* the case of cancellation errors: If we subtract two 16-digit numbers with 13 common leading digits, we are left with 3 digits of valid information. We tend to view the remaining 13 digits as “random.” But really, there is nothing random about what happens inside the computer (we hope!) — the “randomness” will depend on what happened previously...

Accuracy

The **absolute error** of a computation is

$$\|\tilde{f}(\vec{x}) - f(\vec{x})\|$$

and the **relative error** is

$$\frac{\|\tilde{f}(\vec{x}) - f(\vec{x})\|}{\|f(\vec{x})\|}$$

this latter quantity will be our standard measure of error.

If $\tilde{f}$ is a good algorithm, we expect the relative error to be small, of the order $\varepsilon_{\text{mach}}$. We say that $\tilde{f}$ is **accurate** if $\forall \vec{x} \in X$

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

Interpretation: $\mathcal{O}(\varepsilon_{\text{mach}})$

Since all floating point errors are functions of $\varepsilon_{\text{mach}}$ (the relative error in each operation is bounded by $\varepsilon_{\text{mach}}$), the relative error of the algorithm must be a function of $\varepsilon_{\text{mach}}$:

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

The statement

$$e(\varepsilon_{\text{mach}}) = \mathcal{O}(\varepsilon_{\text{mach}})$$

means that $\exists C \in \mathbb{R}^+$ such that

$$e(\varepsilon_{\text{mach}}) \leq C\varepsilon_{\text{mach}}, \quad \text{as} \quad \varepsilon_{\text{mach}} \searrow 0$$

In practice $\varepsilon_{\text{mach}}$ is fixed; the notation means that **if** we were to decrease $\varepsilon_{\text{mach}}$, **then** our error would decrease at least proportionally to $\varepsilon_{\text{mach}}$.

Stability

If the **problem** $f : X \mapsto Y$ is ill-conditioned, then the accuracy goal

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

may be unreasonably ambitious. Instead we aim for **stability**.

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.”

Backward Stability

For many algorithms we can tighten this somewhat vague concept of stability.

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.”

Next: Examples of stable and unstable algorithms;
Stability of Householder triangularization.