Lecture 1: Floating point numbers, Conditioning

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1 Floating-point numbers

1.1 What are floating-point numbers?

The real numbers $\mathbb{R}$ are infinite in two ways:

- the numbers within are unbounded, and
- between any two real numbers that are not equal, there are infinitely many real numbers.

In computation, the second type of infiniteness has many consequences! We don't often need to compute with numbers that are growing unbounded, but we likely often encounter numbers that have relatively small magnitude but require infinite precision to represent. For instance, think of π!

Note that computers necessarily have finite memory and thus cannot exactly represent all real numbers.

> Exercise: How many numbers?
>
> How many real numbers can be represented with 32 bits[1] ("binary digits")?

Answer:

2^{32} – each bit can take on two values, and each bit doubles the the total number of bit strings possible

> Exercise: Which numbers?
>
> Given 32 bits ("binary digits"), which numbers are represented?

Answer:

We don't know! It could be that the bit string is expanded in the usual way – the last bit additively contributes 2^0 or 0, the second to last bit additively contributes 2^1 or 0, the third to last bit additively contributes 2^2 or 0, and so on. However, we could also decide that these bit strings represent these values multiplied by 10. Or we could decide that one of these bit strings represents π.

There are a finite number of real numbers that can be represented in memory, and there are *many* sets of numbers that one can choose to represent.

> Definition: Floating-point numbers
>
> The set $\mathbb{F}$ of **floating-point numbers** consists of zero and all numbers of the form
>
> $$\pm(1+f)\times 2^n,$$
>
> where n is an integer called the **exponent**, and $1+f$ is the **mantissa** or **significand**, in which f is a binary fraction,
>
> $$f=\sum_{i=1}^{d} b_i 2^{-i}, \qquad b_i\in\{0,1\},$$
>
> for a fixed integer d called the binary **precision**.[2]

Note that we may rewrite $f=2^{-d}\sum_{i=1}^{d} b_i 2^{d-i}=2^{-d}z$ where $z\in\{0,1,\cdots,2^d-1\}$.

> Exercise:
>
> How many floating-point numbers are there in $[2^n,2^{n+1})$?

Answer:

There are 2^d floating-point numbers in this interval! For any choice of n, they are enumerated by the set $\{0,1,\cdots,2^d-1\}$.

> Note:
>
> As n grows, the gap between consecutive floating-point numbers also grows!

---

[1] Note: "Bit" was coined by Claude Shannon (of information theory fame – e.g., "Shannon entropy") and attributed to Tukey (a famous statistician)!

[2] This definition is simpler than how numbers are truly represented in the computer. This will be our working definition for class, but to give you a small sense of how things are more complex in reality, we'll dig a bit into the IEEE standards.

Definition: Machine epsilon

For a floating-point set with d binary digits of precision, **machine epsilon** (or *machine precision*) is $\epsilon_{\text{mach}} = 2^{-d}$.

Note that this is the distance between 1 and the smallest element of $\mathbb{F}$ greater than 1, $1 + 2^{-d}$.

Now, remember that an element of $\mathbb{F}$ represents all real numbers closest to it. It will be useful to be able to represent which element of $\mathbb{F}$ represents a given real number. We'll define a function $\text{fl}(x)$ to help us with this map.

Definition: Floating-point rounding function

Given a real number x, the rounding function $\text{fl}(x)$ outputs the element of $\mathbb{F}$ nearest to x.

The distance between consecutive floating-point numbers in $[2^n, 2^{n+1})$ is

$$2^n \epsilon_{\text{mach}} = 2^{n-d}.$$

Thus, for real $x \in [2^n, 2^{n+1})$ we have the bound

$$|\text{fl}(x) - x| \leq \frac{1}{2} 2^n \epsilon_{\text{mach}} \leq \frac{1}{2} \epsilon_{\text{mach}} |x|.$$

---

2 Precision and Accuracy

2.1 Accuracy

The accuracy of an approximation $\tilde{x}$ to the number of interest x. The floating-point number approximation $\tilde{x}$ is represented using d binary digits, but not all of these binary digits may accurately represent (agree) with the number of interest x (which we may be unable to represent exactly as a floating-point number).

Definition:

The **absolute accuracy** of $\tilde{x}$ is $|\tilde{x} - x|$.

Definition:

The **relative accuracy** of $\tilde{x}$ is $\frac{|\tilde{x} - x|}{|x|}$.

Note that absolute accuracy has the same units as x (and may be impacted by the scale of x), while relative accuracy is dimensionless. The number of accurate digits is

$$-\log_{10} \frac{|\tilde{x} - x|}{|x|}.$$

2.2 Example: Approximation to π

```
@show p = 22/7;
```

```
p = 22 / 7 = 3.142857142857143
```

One really cool feature of the Julia programming language is that we can write programs using a broad variety of unicode characters. For instance, below we have used the unicode character π – we get this to appear by typing `\pi` and then the tab button. Many symbol commands from LaTeX work in this same way, and additionally many more symbols can be completed – see the table at https://docs.julialang.org/en/v1/manual/unicode-input/.

```
@show float( );
```

```
float( ) = 3.141592653589793
```

```
acc = abs(p -  )
println("absolute accuracy = $acc")
println("relative accuracy = $(acc/ )")
```

```
absolute accuracy = 0.0012644892673496777
relative accuracy = 0.0004024994347707008
```

Another nice feature of Julia is the `$`, which substitutes the named variable or expression's value into the string. This is sometimes called *interpolation*.

```
println("Number of accurate digits = $(floor(-log10(acc/ )))")
```

```
Number of accurate digits = 3.0
```

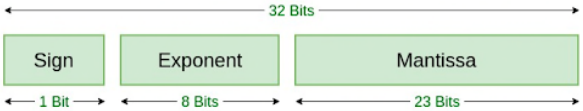
2.3 Precision

The **precision** of a floating-point number is always d binary digits. This is a measure between floating-point numbers.

3 IEEE 754 Standard

3.1 IEEE double and single precision

In 1985, the IEEE set the standard (IEEE 754) for binary and decimal floating point numbers and algorithms for rounding arithmetic operations, which are (generally) followed by all major computer manufacturers.



(a) IEEE single precision

(a) IEEE double precision

Exercise:

1. How many bits would be necessary to represent sign information for a complex number $a + bi$?
2. How many distinct exponents can be represented in double precision and which exponents are they?

Answer:

1. We would need two bits to keep track of the sign of a and the sign of b.

2. In double precision, there are 2^{11} distinct exponents, but we don't know which numbers they are!

The IEEE double precision floating point number has value

$$(-1)^s 2^{c-1023}(1+f),$$

where

- sign s is the binary number 0 or 1
- characteristic c is the binary number given by its bits (in the usual way) and 1023 is subtracted to yield the exponent
- mantissa f is the binary fraction given by its bits (following the "decimal point")

Why do you think 1023 is subtracted from c in the exponent? Note that if we do not shift the exponents in this way, only numbers of magnitude greater than 1 can be represented. Subtracting 1023 (roughly half of the largest value c takes on) means that roughly half of the possible exponents are positive and half are negative.

Note:

In double precision,

$$\epsilon_{\text{mach}} = 2^{-52} \approx 2.2 \times 10^{-16}.$$

Exercise:

Which real numbers are represented by the IEEE double precision number 0 10000000001 $10\cdots0$?

Answer:

1. First, the exact decimal number this represents has

$$c = 1 \times 2^{10} + 0 \times 2^9 + \cdots + 0 \times 2^1 + 1 \times 2^0 = 1024 + 1 = 1025,$$

$$f = 1 \times 2^{-1} + 0 \times 2^{-2} + \cdots + 0 \times 2^{-52},$$

   and so it is $(-1)^0 2^{1025-1023}(1+1/2) = 6$.
2. The next smallest representable number is

$$(-1)^0 2^{1025-1023}(1 + 1/2 - (1/2)^{-52}) = 6 - (1/2)^{50}.$$

3. The next largest representable number is $6 + (1/2)^{50}$.
4. Thus, the interval of real numbers closest to this machine number is

$$(6 - (1/2)^{51}, 6 + (1/2)^{51}).$$

The Julia command for double precision ϵ_{mach} is `eps()`. Recall that this value is proportional to the spacing between adjacent floating-point values at `1.0`.

```
@show eps();
@show eps(1.0);
@show log2(eps());
```

```
eps() = 2.220446049250313e-16
eps(1.0) = 2.220446049250313e-16
log2(eps()) = -52.0
```

We can get values proportional to the spacing at other values by passing them as input to `eps()`.

```
@show eps(1.618);
@show eps(161.8);
```

```
eps(1.618) = 2.220446049250313e-16
eps(161.8) = 2.842170943040401e-14
```

We can also see the next floating-point number larger than a given value using `nextfloat()`.

```
@show nextfloat(161.8);
@show nextfloat(161.8) - 161.8;
```

```
nextfloat(161.8) = 161.80000000000004
nextfloat(161.8) - 161.8 = 2.842170943040401e-14
```

The range[3] of positive values representable in double precision is

```
@show floatmin(), floatmax();
```

```
(floatmin(), floatmax()) = (2.2250738585072014e-308, 1.7976931348623157e308)
```

Like other languages, Julia has different types, which is very important for numerical computing (as we'll see in more detail later)!

```
@show typeof(1);
@show typeof(1.0);
```

```
typeof(1) = Int64
typeof(1.0) = Float64
```

The standard floating-point representation is `Float64`, which is IEEE double precision using 64 bits. We can ask Julia to show us the bits using `bitstring`.

```
[bitstring(1.0), bitstring(-1.0), bitstring(2.0)]
```

```
3-element Vector{String}:
 "0011111111110000000000000000000000000000000000000000000000000000"
 "1011111111110000000000000000000000000000000000000000000000000000"
 "0100000000000000000000000000000000000000000000000000000000000000"
```

> Exercise: What do you notice?
>
> What do you notice about the bitstrings above?

Answer:

- The first bit gives the sign of the number.
- The next 11 bits determine the exponent (remember to subtract 1023).
- The last 52 bits determine the mantissa (binary fraction).

Note that the representation of `Int64` is different!

[3] A common mistake made is to think that ϵ_{mach} is the smallest magnitude floating-point number. It is only the smallest *relative to 1.0*. The exponent limits the scaling of values – the distance between floating-point numbers (governed by the mantissa) is smallest when the values themselves (governed by the exponent) are smallest.

```
[bitstring(1), bitstring(-1), bitstring(2), bitstring(-2)]
```

```
4-element Vector{String}:
 "0000000000000000000000000000000000000000000000000000000000000001"
 "1111111111111111111111111111111111111111111111111111111111111111"
 "0000000000000000000000000000000000000000000000000000000000000010"
 "1111111111111111111111111111111111111111111111111111111111111110"
```

Julia can also give the sign, exponent, and significand in decimal. Note that the significand is the entire floating-number without the exponential; that is $(-1)^s(1+f)$.

```
x = -1.0
@show sign(x), exponent(x), significand(x);
```

```
(sign(x), exponent(x), significand(x)) = (-1.0, 0, -1.0)
```

```
x = 0.125
@show sign(x), exponent(x), significand(x);
```

```
(sign(x), exponent(x), significand(x)) = (1.0, -3, 1.0)
```

The definition of floating-point numbers $\mathbb{F}$ given on slide 5 did not put limits on the exponent, but in double precision we have $-1022 \leq n \leq 1023$.

- Values larger than 2^{1024} (either input or computed) are said to *overflow* and will be instead represented by the value `Inf` in memory.
- Values smaller than 2^{-1022} are said to *underflow* to zero.

Overflow and underflow can cause very real, and very disastrous problems. In 1996, the European Space Agency launched their $7 billion Arianne 5 rocket, which they had spent 10 years developing. It exploded less than 40 secons into the the flight sequence. The 'Inertial Reference System' software that used calculations involving the velocity of the rocket to manage the flight path attempted to convert a bit of data from 64-bit floating point to 16-bit signed integer. Due to the higher velocity of the Arianne 5 rocket over previous versions, the bit of data to be converted had value greater than 2^{15}, which caused overflow and the guidance system to shut down.

You should also be aware of one more double-precision value: `NaN`, which stand for *not a number*. This value is adopted after undefined arithmetic operations (like division by zero or division by values in underflow).

4 Floating-point Arithmetic

4.1 Computer arithmetic

In a computer, arithmetic operations operate on floating-point numbers and return floating-point results. IEEE standards define machine-analog operations for the arithmetic operations $+, -, \times, \div, \sqrt{\cdot}$, etc. Perhaps the most important thing for you to know is that while operations $+, -, \times, /$ produce *exact* results, the machine-analog operations, which we will denote $\oplus, \ominus, \otimes, \oslash$, are not guaranteed to do so.

Recall that there is no double-precision number between 1 and $1 + \epsilon_{\text{mach}}$. This causes the following loss of accuracy.

```
e = eps()/2
(1.0 + e) - 1.0
```

```
0.0
```

However, in the interval $[1/2, 1)$, floating-point numbers have spacing $\epsilon_{\text{mach}}/2$, so $1-\epsilon_{\text{mach}}/2$ and its negative are exactly representable. Rewriting the calculation above results in a very different, and exactly correct, result!

```
1.0 + (e - 1.0)
```

```
1.1102230246251565e-16
```

Computer addition is not associative! This, amongst the many other surprising facts about computer arithmetic, emphasizes how important it is to think through computer implementations of even simple algorithms. The IEEE standard for floating-point addition, alone, is several pages long!

> Fact
>
> Two mathematically equivalent results need not be equal when computed in floating point arithmetic. One would hope that they be relatively close together.

An important job of one working in scientific computation is to ensure that results are computed in such a way that they are close together!

5 Problems and Conditioning

5.1 Example

Think about the problem of subtracting 1 from a number x; this result is given by the function $f(x) = x - 1$. On a computer, x is represented by $\text{fl}(x)$ and by the previous inequality $|\text{fl}(x) - x| \leq \frac{1}{2}\epsilon_{\text{mach}}|x|$ we have $\text{fl}(x) = x(1+\epsilon)$ for some $|\epsilon| < \epsilon_{\text{mach}}/2$. Also, $\text{fl}(1) = 1$, since it can be represented exactly.

Even if the floating-point arithmetic addition is exact, so $x \ominus 1 = x(1+\epsilon) - 1$, the relative error in this result is

$$\frac{|(x + \epsilon x - 1) - (x - 1)|}{|x - 1|} = \frac{|\epsilon x|}{|x - 1|}.$$

This relative error can be unboundedly poor by taking x very close to 1.

> Definition:
>
> **Subtractive cancellation** is a loss of accuracy that occurs when two numbers add or subtract to give a result that is much smaller in magnitude than the inputs. It is one of the most common mechanisms for causing dramatic growth of errors in floating-point computations!

Subtractive cancellation renders some of the digits in our floating-point representations essentially meaningless, since they are zeroed in our calculation. You may have encountered this previously. Consider adding -1.0012 to 1.0000, both of which are results rounded to five decimal digits. The result is -0.0012, which has only two digits. Three digits were "lost" in this calculation, and no algorithm could save them as we had cut the inputs at a fixed number of digits.

5.2 Problems

Consider a problem – this is a calculation or task for which you might write an algorithm. We'll represent a problem as a function f that maps a real data value x to a real result $f(x)$, and denote this $f : \mathbb{R} \to \mathbb{R}$. Everything here denotes exact calculations – data x is represented exactly and the exact result $f(x)$ is computed exactly.

In a computer, the problem f will be approximated in floating-point. Here the data x is represented as an *input* $\tilde{x} = \text{fl}(x)$.

Realistically the calculations required to solve the problem f will also be inexact and so we might instead solve a different problem $\tilde{f}$. Here the *output* $\tilde{f}(x)$ could be different from the result $f(x)$.

5.3 Conditioning

Setting aside the sources of error in the problem calculations, we'll consider the ratio of the relative errors of the result and the data,

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

This ratio gives us a sense of how much the effect of the error in the representation of the data has on the solution of the problem.

> Exercise: Rewrite this expression
>
> Show that for the floating-point approximation to x, $\tilde{x}$, for some $|\epsilon| \leq \epsilon_{\text{mach}}/2$, this ratio is equal to
>
> $$\frac{|f(x) - f(x+\epsilon x)|}{|\epsilon f(x)|}.$$

Answer:

We have $\tilde{x} = x(1+\epsilon)$ and thus

$$\frac{|f(x) - f(\tilde{x})||x|}{|f(x)||x-\tilde{x}|} = \frac{|f(x) - f(x+\epsilon x)||x|}{|f(x)||\epsilon x|} = \frac{|f(x) - f(x+\epsilon x)|}{|\epsilon f(x)|}.$$

5.4 Condition Number

Now, think about what would happen in a perfect computer where the floating-point representation is perfect, $\epsilon \to 0$.

> Definition: Condition number for scalar function
>
> The relative **condition number** of a scalar function $f(x)$ is
>
> $$\kappa_f(x) = \lim_{\epsilon \to 0} \frac{|f(x) - f(x+\epsilon x)|}{|\epsilon f(x)|}.$$

Note that this is the limit of the ratio of the error in the result (of the problem) to the input error, as the input error goes to 0. It does not depend upon the computer, or the algorithm for solving the problem, only the ideal data x and the problem f.

> Exercise: Rewrite this expression
>
> Assuming that f has a continuous derivative f', show that $\kappa_f(x) = \left|\frac{xf'(x)}{f(x)}\right|$.

Answer:

Using the definition of the derivative, we have

$$\kappa_f(x) = \lim_{\epsilon \to 0} \left|\frac{f(x+\epsilon x) - f(x)}{\epsilon f(x)}\right| = \left|\frac{f(x+\epsilon x) - f(x)}{\epsilon x}\right| \left|\frac{x}{f(x)}\right| = \left|\frac{xf'(x)}{f(x)}\right|.$$

Using the previous exercise, we see that the condition number for the problem of subtracting a constant number c from data x, $f(x) = x - c$, has condition number

$$\kappa_f(x) = \left| \frac{(x)(1)}{x - c} \right| = \frac{|x|}{|x - c|}$$

which is large when $|x| \gg |x - c|$.

> Note:
>
> This is indicative of the risk of subtractive cancellation when x is nearby to c!

> Exercise: What is the condition number?
>
> Calculate the condition number of $g(x) = cx$.

Answer:

We have

$$\kappa_g(x) = \left| \frac{(x)(c)}{cx} \right| = 1.$$

Multiplication has the same relative error in the result as in the data!

5.5 Estimating Error

If $|\epsilon|$ is small, we expect

$$\left| \frac{f(x + \epsilon x) - f(x)}{f(x)} \right| \approx \kappa_f(x)|\epsilon|.$$

When the data x is perturbed by a small amount ϵ, the relative error in the result is magnified by a factor of $\kappa_f(x)$.

> Fact:
>
> If $\kappa_f(x) \approx 10^d$, then we expect to lose up to d decimal digits of accuracy in computing $f(x)$ from x.

When the condition number of a problem is large, we cannot expect errors in the result to remain comparable in size to roundoff error. This type of problem is called **ill-conditioned**. We say a problem f is ill-conditioned when $\kappa_f(x) \gg 1$. There is no strict threshold for this inequality. It is important to think about the repercussion of your problem's condition number!

Some problems, such as $f(x) = \sqrt{x}$, can have a condition number less than 1. However, every result in floating-point arithmetic is subject to rounding error at the relative level of ϵ_{mach}, so in practice, $\kappa_f(x) < 1$ is no different from $\kappa_f(x) = 1$.

5.6 Case Study: Conditioning

We're going to consider the problem of calculating roots of a quadratic polynomial; that is finding values t such that $at^2 + bt + c = 0$. We'll start first by considering the *conditioning* of the problem, which we might write $f([a, b, c]) = [r_1, r_2]$ for coefficients a, b, c and roots r_1, r_2.

Since we've been thinking of conditioning for problems which are scalar functions, let's think only of how r_1 changes as we vary a and hold b and c fixed, that is $f(a) = r_1$.

Now, noting that $ar_1^2 + br_1 + c = 0$, we may differentiate with respect to a and get

$$r_1^2 + 2ar_1\frac{dr_1}{da} + b\frac{dr_1}{da} = 0.$$

Solving this for the derivative, we have $\frac{dr_1}{da} = \frac{-r_1^2}{2ar_1+b}$, and thus, the conditioning is

$$\kappa_f(a) = \left|\frac{a}{r_1}\frac{dr_1}{da}\right| = \left|\frac{ar_1}{2ar_1+b}\right| = \left|\frac{r_1}{r_1-r_2}\right|.$$

Here, we have used the quadratic formula and the fact that

$$\frac{|2ar_1+b|}{|a|} = \frac{|\sqrt{b^2-4ac}|}{|a|} = |r_1 - r_2|.$$

Thus, the condition number of a root can be arbitrarily large!

> Fact:
>
> Roots of polynomials are ill-conditioned with respect to changes in the polynomial coefficients when the roots are much closer to one another than the origin.

If a polynomial has a repeated root, then the condition number of the polynomial is formally infinite.

The polynomial $p(x) = \frac{1}{3}(x-1)(x-1-\epsilon)$ has roots 1 and $1+\epsilon$. For small values of ϵ, the roots are ill-conditioned.

```
  = 1e-6
a,b,c = 1/3, (-2- )/3, (1+ )/3;
```

We can use unicode ϵ as a variable by typing `\epsilon` and then hitting tab. Additionally, we can make multiple variable assignments at once, as in Line 2 above. The `;` suppresses the output from the executed Julia code.

We can use the quadratic formula to compute the roots (this is an algorithm)!

```
d = sqrt(b^2 - 4a*c)
r  = (-b-d)/(2a)
r  = (-b+d)/(2a)
(r ,r )
```

```
(0.9999999998251499, 1.0000010001748503)
```

To get r_1 above, we type `r\_1` and hit Tab. Let's now look at the relative error in r_1!

```
abs(r -(1+ ))/(1+ )
```

```
1.748501815656639e-10
```

Since the condition number is proportional to $1/2\epsilon$, we estimate the roundoff in the data can grow in the result to be approximately $\epsilon_{\text{mach}}/2\epsilon$.

```
eps()/2
```

```
1.1102230246251565e-10
```