33. Interval arithmetic

Last time

- Spectral methods for ODE boundary-value problems

Goals for today

- Interval arithmetic
- Need for interval arithmetic
- Basic properties

Motivation: Ground state of atomic cluster

- N atoms at positions $\mathbf{x}_i \in \mathbb{R}^3$
- **Interaction potential** $V(r_{ij})$ between pairs
- Ground state: Minimize **potential energy**

$$V(\mathbf{x}_1, \ldots, \mathbf{x}_N) := \sum_{i=1}^{N} \sum_{j>i} V(r_{ij})$$

- $r_{ij} := \|\mathbf{x}_i - \mathbf{x}_j\|$ is distance between atoms i and j

Lennard-Jones potential

- Standard model of interaction between argon atoms:

$$V(r) := 4\left(\frac{1}{r^{12}} - \frac{1}{r^{6}}\right)$$

- Problem: There are *lots* of local minima
- Estimated to grow like $O(e^N)$
- To find the ground state we need **global optimization**

Standard floats are not always good enough

- Example by Siegried Rump: Calculate

$$f(a,b) = 333.75b^6 + a^2(11a^2b^2 - b^6 - 121b^4 - 2) + 5.5b^8 + a/$$

at $a = 77617$ and $b = 33096$

Standard floats are not always good enough

- Example by Siegried Rump: Calculate

$$f(a,b) = 333.75b^6 + a^2(11a^2b^2 - b^6 - 121b^4 - 2) + 5.5b^8 + a/$$

  at $a = 77617$ and $b = 33096$

- Something weird happens when trying `Float32`, `Float64` and `BigFloat`

Standard floats are not always good enough

- Example by Siegried Rump: Calculate

$$f(a,b) = 333.75b^6 + a^2(11a^2b^2 - b^6 - 121b^4 - 2) + 5.5b^8 + a/$$

  at $a = 77617$ and $b = 33096$

- Something weird happens when trying `Float32`, `Float64` and `BigFloat`
- Get totally different answers
- Which is correct?

Standard floats are not always good enough II

- Example by William Kahan: Consider

$$f(x) = \frac{1}{50} \log |3(1-x)+1| + x^2 + 1$$

- Looks uncomplicated if you sample it at many points to draw it

Standard floats are not always good enough II

- Example by William Kahan: Consider

$$f(x) = \frac{1}{50} \text{log} \, |3(1-x)+1| + x^2 + 1$$

- Looks uncomplicated if you sample it at many points to draw it
- Is it really that uncomplicated?

What is 0.1 anyway?

- When I type `0.1`, what does it mean?

What is 0.1 anyway?

- When I type `0.1`, what does it mean?
- It's a floating-point `Float64` value. Which value?

What is 0.1 anyway?

- When I type `0.1`, what does it mean?
- It's a floating-point `Float64` value. Which value?
- Look at its exact value:

```
big(0.1)
```

What is 0.1 anyway?

- When I type `0.1`, what does it mean?
- It's a floating-point `Float64` value. Which value?
- Look at its exact value:

```
big(0.1)
```

- Look at its bits (binary representation):

```
bitstring(0.1)
```

Calculating with sets

- Can we calculate with *sets* of real numbers instead?

Calculating with sets

- Can we calculate with *sets* of real numbers instead?
- E.g. “small” sets containing non-representable numbers like 0.1 or π

Calculating with sets

- Can we calculate with *sets* of real numbers instead?
- E.g. “small” sets containing non-representable numbers like 0.1 or π
- Or larger sets

Calculating with sets

- Can we calculate with *sets* of real numbers instead?
- E.g. “small” sets containing non-representable numbers like 0.1 or π
- Or larger sets
- What does it mean to “calculate with a set”?
- What are basic questions about function f on set X?

Range of a function

- Basic questions concern **range** of a function f on set X

Range of a function

- Basic questions concern **range** of a function f on set X
- range$(f; X) := \{f(x) : x \in X\}$

Range of a function

- Basic questions concern **range** of a function f on set X
- range$(f; X) := \{f(x) : x \in X\}$
- Set of all possible output values for inputs in X

Range of a function

- Basic questions concern **range** of a function f on set X
- range$(f; X) := \{f(x) : x \in X\}$
- Set of all possible output values for inputs in X
- Mathematics assumes that the range is accessible

Range of a function

- Basic questions concern **range** of a function f on set X
- $\text{range}(f; X) := \{f(x) : x \in X\}$
- Set of all possible output values for inputs in X
- Mathematics assumes that the range is accessible
- But can we **calculate** the range of a function?

Range II

- Conceptually easy: Find minimum and maximum over X

Range II

- Conceptually easy: Find minimum and maximum over X
- That is itself a difficult optimization problem!

Range II

- Conceptually easy: Find minimum and maximum over X
- That is itself a difficult optimization problem!
- Can we obtain *some* information about range more easily?

Range II

- Conceptually easy: Find minimum and maximum over X
- That is itself a difficult optimization problem!
- Can we obtain *some* information about range more easily?
- What would be most useful?
- What are simplest sets to think about?

Intervals

- Range of real numbers
- Simplest: (closed) **interval** on real line:

$$X = [a..b] = \{a \leq x \leq b : x \in \mathbb{R}\}$$

- (Standard notation $[a, b])

Intervals

- Range of real numbers
- Simplest: (closed) **interval** on real line:

$$X = [a..b] = \{a \leq x \leq b : x \in \mathbb{R}\}$$

- (Standard notation $[a, b])
- Infinite (uncountable) number of elements x in set X

Intervals

- Range of real numbers
- Simplest: (closed) **interval** on real line:

$$X = [a..b] = \{a \leq x \leq b : x \in \mathbb{R}\}$$

- (Standard notation $[a, b])
- Infinite (uncountable) number of elements x in set X
- How can we represent an interval X in Julia?

Intervals in Julia

- Define new `SimpleInterval` type:

```julia
struct SimpleInterval
    inf::Float64
    sup::Float64
end
```

Intervals in Julia

- Define new `SimpleInterval` type:

```
struct SimpleInterval
    inf::Float64
    sup::Float64
end
```

- And set operations, e.g.

```
Base.in(a::Real, X::SimpleInterval) = X.inf ≤ a ≤ X.sup
```

Intervals in Julia

- Define new `SimpleInterval` type:

```
struct SimpleInterval
    inf::Float64
    sup::Float64
end
```

- And set operations, e.g.

```
Base.in(a::Real, X::SimpleInterval) = X.inf ≤ a ≤ X.sup
```

- Can we define *arithmetic* on these *sets*?

Functions on intervals

- Given an interval X
- Suppose f is a function like $f(x) = x^2$

Functions on intervals

- Given an interval X
- Suppose f is a function like $f(x) = x^2$
- Can we define $f(X)$?
- What should this mean?

Functions on intervals

- Given an interval X
- Suppose f is a function like $f(x) = x^2$
- Can we define $f(X)$?
- What should this mean?
- How should we calculate it?

Functions on intervals

- Given an interval X
- Suppose f is a function like $f(x) = x^2$
- Can we define $f(X)$?
- What should this mean?
- How should we calculate it?
- Goal: Find **range** of f over X, i.e. set of possible values

Functions on intervals II

- Apply f to X by applying f to *each element of* X
- Will give a new set as output
- Obviously *impossible* to do this since too many elements
- So instead use maths to calculate *what answer should be*

Example: Squaring

- Let's think about $f(x) = x^2$
- With $X = [1..2]$
- What is result of squaring every element?
- So how can we define X^2?
- What about $[-1..2]^2$?

Squaring II

- General rule:

$$
\begin{aligned}
[a,b] &:= [a^2, b^2] \quad \text{if } a \geq 0 \\
&:= [0, \max(a^2, b^2)] \quad \text{if } a < 0 \text{ and } b > 0 \\
&:= [b^2, a^2] \quad \text{if } a < b < 0
\end{aligned}
$$

Example: Addition

- How should we define $X + Y$ for intervals X and Y?
- Want to add any x and y with $x \in X$ and $y \in Y$
- Problem: What is $[0..1] - [0..1]$?

Application: Finding roots

- Define $f(x) = x^2 - 2$
- Calculate for $X = [3..4]$
- Get $f(X) = [7..14]$
- This does not contain 0
- Hence $0 \notin \text{range}(f; X)$
- So *there is no root of* f *in* X

Review

- Defined arithmetic on intervals
- Applications to root finding and global optimization