Gaussian Elimination (+ Numerics)

Geometric Algorithms
Lecture 4

CAS CS 132

Practice Problem

$$
\begin{aligned}
x + z &= 1\\
x + y + 3z &= 3\\
x - y - z &= -1
\end{aligned}
$$

Write down the general forms solution of the above linear system.

Solution

$$x + z = 1$$
$$x + y + 3z = 3$$
$$x - y - z = -1$$

Objectives

1. (Finally) discuss Gaussian elimination
2. Think more carefully about number representations
3. Look at the consequences of floating point representations
4. Introduce NumPy and talk about best best practices

Keywords

`forward elimination`

`back substitution`

`floating point numbers`

`IEEE-754`

`relative error`

`numpy.isclose`

`ill-conditioned problems`

Defining the Gaussian Elimination (GE) Algorithm

At a High Level

At a High Level

```
eliminations + back–substitution
```

At a High Level

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we've already done this

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but we'll take one step further and write down the algorithm as <u>pseudocode</u>

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but we'll take one step further and write down the algorithm as <u>pseudocode</u>

Keep in mind. How do we turn our intuitions into a formal procedure?

A Word of Warning

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The goal is not to understand it entirely, but to get enough intuition to emulate it.

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You should roughly use Gaussian Elimination when solving a system by hand.

demo

(step–throughs)

The Algorithm

Gaussian Elimination (Specification)

```
FUNCTION GE(A):
  # INPUT: m × n matrix A
  # OUTPUT: equivalent m × n RREF matrix
  ...
```

Gaussian Elimination (High Level)

```
FUNCTION fwd_elim(A):
  # INPUT: m × n matrix A
  # OUTPUT: equivalent m × n echelon form matrix
  ...

FUNCTION back_sub(A):
  # INPUT: m × n echelon form matrix A
  # OUTPUT: equivalent m × n RREF matrix
  ...

FUNCTION GE(A):
  RETURN back_sub(fwd_elim(A))
```

Elimination Stage

Elimination Stage (High Level)

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Input: matrix A of size $m \times n$

Output: echelon form of A

Elimination Stage (High Level)

Input: matrix A of size $m \times n$

Output: echelon form of A

starting at the top left and move down, find a leading entry and eliminate it from latter equations

Edge cases

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What if the first equation doesn't have the variable x_1?

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Swap rows with an equation that does.

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Swap rows with an equation that does.

What if *none* of the equations have the variable x_1?

Edge cases

What if the first equation doesn't have the variable x_1?

Swap rows with an equation that does.

What if *none* of the equations have the variable x_1?

Find the *leftmost* variable which appears in *any* of the remaining equations.

Elimination Stage (Pseudocode)

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```
FUNCTION fwd_elim(A):
```

Elimination Stage (Pseudocode)

```
FUNCTION fwd_elim(A):
  FOR [i from 1 to m]: # for each row from top to bottom
```

Elimination Stage (Pseudocode)

```
FUNCTION fwd_elim(A):
  FOR [i from 1 to m]: # for each row from top to bottom
    IF [rows i...m are all-zeros]: # if remaining rows are zero
```

Elimination Stage (Pseudocode)

```
FUNCTION fwd_elim(A):
  FOR [i from 1 to m]: # for each row from top to bottom
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Elimination Stage (Pseudocode)

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FUNCTION fwd_elim(A):
  FOR [i from 1 to m]: # for each row from top to bottom
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    ELSE:
```

Elimination Stage (Pseudocode)

```
FUNCTION fwd_elim(A):
  FOR [i from 1 to m]: # for each row from top to bottom
    IF [rows i...m are all-zeros]: # if remaining rows are zero
      RETURN A
    ELSE:
      (j, k) ← [position of leftmost entry in the rows i...m]
```

Elimination Stage (Pseudocode)

```
FUNCTION fwd_elim(A):
  FOR [i from 1 to m]: # for each row from top to bottom
    IF [rows i...m are all-zeros]: # if remaining rows are zero
      RETURN A
    ELSE:
      (j, k) ← [position of leftmost entry in the rows i...m]
      [swap row i and row j]
```

Elimination Stage (Pseudocode)

```
FUNCTION fwd_elim(A):
  FOR [i from 1 to m]: # for each row from top to bottom
    IF [rows i...m are all-zeros]: # if remaining rows are zero
      RETURN A
    ELSE:
      (j, k) ← [position of leftmost entry in the rows i...m]
      [swap row i and row j]
      FOR [l from i + 1 to m]: # for all remaining rows
```

Elimination Stage (Pseudocode)

```
FUNCTION fwd_elim(A):
  FOR [i from 1 to m]: # for each row from top to bottom
    IF [rows i...m are all-zeros]: # if remaining rows are zero
      RETURN A
    ELSE:
      (j, k) ← [position of leftmost entry in the rows i...m]
      [swap row i and row j]
      FOR [l from i + 1 to m]: # for all remaining rows
        [zero out A[l, k] using a replacement operation]
```

Elimination Stage (Pseudocode)

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FUNCTION fwd_elim(A):
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      [swap row i and row j]
      FOR [l from i + 1 to m]: # for all remaining rows
        [zero out A[l, k] using a replacement operation]
  RETURN A
```

Elimination Stage (Example)

$$\begin{bmatrix} 0 & 3 & -6 & 6 & 4 & -5 \\ 3 & -7 & 8 & -5 & 8 & 9 \\ 3 & -9 & 12 & -9 & 6 & 15 \end{bmatrix}$$

Elimination Stage (Example)

$$\begin{array}{r} \\ \\ \text{leftmost nonzero entry} \end{array} \begin{bmatrix} 0 & 3 & -6 & 6 & 4 & -5 \\ 3 & -7 & 8 & -5 & 8 & 9 \\ \boxed{3} & -9 & 12 & -9 & 6 & 15 \end{bmatrix}$$

Elimination Stage (Example)

$$\begin{array}{r} \\ \\ \text{leftmost nonzero entry} \end{array} \begin{bmatrix} 0 & 3 & -6 & 6 & 4 & -5 \\ 3 & -7 & 8 & -5 & 8 & 9 \\ \boxed{3} & -9 & 12 & -9 & 6 & 15 \end{bmatrix}$$

Swap R_1 and R_3

Elimination Stage (Example)

$$\begin{bmatrix} 3 & -9 & 12 & -9 & 6 & 15 \\ 3 & -7 & 8 & -5 & 8 & 9 \\ 0 & 3 & -6 & 6 & 4 & -5 \end{bmatrix}$$

Elimination Stage (Example)

$$\begin{array}{r} \\ \texttt{next entry to zero} \\ \\ \end{array} \begin{bmatrix} 3 & -9 & 12 & -9 & 6 & 15 \\ 3 & -7 & 8 & -5 & 8 & 9 \\ 0 & 3 & -6 & 6 & 4 & -5 \end{bmatrix}$$

Elimination Stage (Example)

$$\begin{array}{c} \\ \texttt{next entry to zero} \\ \\ \end{array} \begin{bmatrix} 3 & -9 & 12 & -9 & 6 & 15 \\ 3 & -7 & 8 & -5 & 8 & 9 \\ 0 & 3 & -6 & 6 & 4 & -5 \end{bmatrix}$$

$R_3 \leftarrow R_3 - R_1$

Elimination Stage (Example)

$$\begin{bmatrix} 3 & -9 & 12 & -9 & 6 & 15 \\ 0 & 2 & -4 & 4 & 2 & -6 \\ 0 & 3 & -6 & 6 & 4 & -5 \end{bmatrix}$$

Elimination Stage (Example)

leftmost nonzero entry

$$\begin{bmatrix} 3 & -9 & 12 & -9 & 6 & 15 \\ 0 & 2 & -4 & 4 & 2 & -6 \\ 0 & 3 & -6 & 6 & 4 & -5 \end{bmatrix}$$

Elimination Stage (Example)

leftmost
nonzero
entry

$$\begin{bmatrix} 3 & -9 & 12 & -9 & 6 & 15 \\ 0 & \boxed{2} & -4 & 4 & 2 & -6 \\ 0 & 3 & -6 & 6 & 4 & -5 \end{bmatrix}$$

swap R_2 with R_2

Elimination Stage (Example)

$$\begin{bmatrix} 3 & -9 & 12 & -9 & 6 & 15 \\ 0 & 2 & -4 & 4 & 2 & -6 \\ 0 & 3 & -6 & 6 & 4 & -5 \end{bmatrix}$$

Elimination Stage (Example)

$$\begin{array}{r} \\ \\ \texttt{next entry to zero} \end{array} \begin{bmatrix} 3 & -9 & 12 & -9 & 6 & 15 \\ 0 & 2 & -4 & 4 & 2 & -6 \\ 0 & \boxed{3} & -6 & 6 & 4 & -5 \end{bmatrix}$$

Elimination Stage (Example)

$$\begin{array}{r}\\ \\ \texttt{next entry to zero}\end{array}\begin{bmatrix} 3 & -9 & 12 & -9 & 6 & 15 \\ 0 & 2 & -4 & 4 & 2 & -6 \\ 0 & \boxed{3} & -6 & 6 & 4 & -5 \end{bmatrix}$$

$$R_3 \leftarrow R_3 - \frac{3R_2}{2}$$

Elimination Stage (Example)

$$\begin{bmatrix} 3 & -9 & 12 & -9 & 6 & 15 \\ 0 & 2 & -4 & 4 & 2 & -6 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{bmatrix}$$

Elimination Stage (Example)

$$\begin{array}{cc}
 & \\
 & \left[\begin{array}{cccccc} 3 & -9 & 12 & -9 & 6 & 15 \\ 0 & 2 & -4 & 4 & 2 & -6 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{array}\right] \\
\texttt{leftmost nonzero entry} &
\end{array}$$

Elimination Stage (Example)

$$\begin{array}{r c}
 & \begin{bmatrix} 3 & -9 & 12 & -9 & 6 & 15 \\ 0 & 2 & -4 & 4 & 2 & -6 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{bmatrix}
\end{array}$$

leftmost nonzero entry

swap R_3 with R_3

Elimination Stage (Example)

$$\begin{bmatrix} 3 & -9 & 12 & -9 & 6 & 15 \\ 0 & 2 & -4 & 4 & 2 & -6 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{bmatrix}$$

Elimination Stage (Example)

$$\begin{bmatrix} 3 & -9 & 12 & -9 & 6 & 15 \\ 0 & 2 & -4 & 4 & 2 & -6 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{bmatrix}$$

done with elimination stage
going to back substitution stage

Back Substitution Stage

Back Substitution Stage (High Level)

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Input: matrix A of size $m \times n$ in echelon form

Output: reduced echelon form of A

Back Substitution Stage (High Level)

Input: matrix A of size $m \times n$ in echelon form

Output: reduced echelon form of A

scale pivot positions and eliminate the variables for that column from the other equations

Back Substitution (Psuedocode)

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```
FUNCTION back_sub(A):
```

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FUNCTION back_sub(A):
  FOR [i from 1 to m]: # for each row from top to bottom
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FUNCTION back_sub(A):
  FOR [i from 1 to m]: # for each row from top to bottom
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      j ← index of leading entry of row i
```

Back Substitution (Psuedocode)

```
FUNCTION back_sub(A):
  FOR [i from 1 to m]: # for each row from top to bottom
    IF [row i has a leading entry]:
      j ← index of leading entry of row i
      $R_i$(A) ← $R_i$(A) / A[i, j] # divide by leading entry
```

Back Substitution (Psuedocode)

```
FUNCTION back_sub(A):
  FOR [i from 1 to m]: # for each row from top to bottom
    IF [row i has a leading entry]:
      j ← index of leading entry of row i
      $R_i$(A) ← $R_i$(A) / A[i, j] # divide by leading entry
      FOR [k from 1 to i - 1]: # for the rows above the current one
```

Back Substitution (Psuedocode)

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  FOR [i from 1 to m]: # for each row from top to bottom
    IF [row i has a leading entry]:
      j ← index of leading entry of row i
      $R_i$(A) ← $R_i$(A) / A[i, j] # divide by leading entry
      FOR [k from 1 to i − 1]: # for the rows above the current one
        $R_k$(A) ← $R_k$(A) − R[k, j] ∗ $R_i$(A)
        # zero out R[k, j] above the leading entry
```

Back Substitution (Psuedocode)

```
FUNCTION back_sub(A):
  FOR [i from 1 to m]: # for each row from top to bottom
    IF [row i has a leading entry]:
      j ← index of leading entry of row i
      $R_i$(A) ← $R_i$(A) / A[i, j] # divide by leading entry
      FOR [k from 1 to i - 1]: # for the rows above the current one
        $R_k$(A) ← $R_k$(A) - R[k, j] ∗ $R_i$(A)
        # zero out R[k, j] above the leading entry
  RETURN A
```

You will have to implement this part in HW2...

Gaussian Elimination (Example)

$$\begin{bmatrix} 3 & -9 & 12 & -9 & 6 & 15 \\ 0 & 2 & -4 & 4 & 2 & -6 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{bmatrix}$$

Gaussian Elimination (Example)

$$\begin{array}{cc} \texttt{pivot position} & \begin{bmatrix} \boxed{3} & -9 & 12 & -9 & 6 & 15 \\ 0 & 2 & -4 & 4 & 2 & -6 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{bmatrix} \end{array}$$

Gaussian Elimination (Example)

$$\begin{array}{c c}
\texttt{pivot position} & \left[\begin{array}{cccccc} 3 & -9 & 12 & -9 & 6 & 15 \\ 0 & 2 & -4 & 4 & 2 & -6 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{array}\right]
\end{array}$$

$R_1 \leftarrow R_1 \,/\, 3$

Gaussian Elimination (Example)

$$\begin{bmatrix} 1 & -3 & 4 & -3 & 2 & 5 \\ 0 & 2 & -4 & 4 & 2 & -6 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{bmatrix}$$

Gaussian Elimination (Example)

$$\begin{array}{c c}
 & \\
\texttt{pivot position} & \left[\begin{array}{cccccc} 1 & -3 & 4 & -3 & 2 & 5 \\ 0 & 2 & -4 & 4 & 2 & -6 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{array}\right] \\
 &
\end{array}$$

Gaussian Elimination (Example)

$$\begin{array}{r} \\ \text{pivot position} \\ \\ \end{array} \begin{bmatrix} 1 & -3 & 4 & -3 & 2 & 5 \\ 0 & 2 & -4 & 4 & 2 & -6 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{bmatrix}$$

$R_2 \leftarrow R_2 \,/\, 2$

Gaussian Elimination (Example)

$$\begin{bmatrix} 1 & -3 & 4 & -3 & 2 & 5 \\ 0 & 1 & -2 & 2 & 1 & -3 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{bmatrix}$$

Gaussian Elimination (Example)

```
next entry
 to zero
```

$$\begin{bmatrix} 1 & -3 & 4 & -3 & 2 & 5 \\ 0 & 1 & -2 & 2 & 1 & -3 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{bmatrix}$$

Gaussian Elimination (Example)

next entry to zero

$$\begin{bmatrix} 1 & \boxed{-3} & 4 & -3 & 2 & 5 \\ 0 & 1 & -2 & 2 & 1 & -3 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{bmatrix}$$

$$R_1 \leftarrow R_1 + 3R_2$$

Gaussian Elimination (Example)

$$\begin{bmatrix} 1 & 0 & -2 & 3 & 5 & -4 \\ 0 & 1 & -2 & 2 & 1 & -3 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{bmatrix}$$

Gaussian Elimination (Example)

pivot position

$$\begin{bmatrix} 1 & 0 & -2 & 3 & 5 & -4 \\ 0 & 1 & -2 & 2 & 1 & -3 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{bmatrix}$$

Gaussian Elimination (Example)

pivot position

$$\begin{bmatrix} 1 & 0 & -2 & 3 & 5 & -4 \\ 0 & 1 & -2 & 2 & 1 & -3 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{bmatrix}$$

$R_3 \leftarrow R_3 \ / \ 1$

Gaussian Elimination (Example)

$$\begin{bmatrix} 1 & 0 & -2 & 3 & 5 & -4 \\ 0 & 1 & -2 & 2 & 1 & -3 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{bmatrix}$$

Gaussian Elimination (Example)

next entry
to zero

$$\begin{bmatrix} 1 & 0 & -2 & 3 & 5 & -4 \\ 0 & 1 & -2 & 2 & 1 & -3 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{bmatrix}$$

Gaussian Elimination (Example)

next entry
to zero

$$\begin{bmatrix} 1 & 0 & -2 & 3 & 5 & -4 \\ 0 & 1 & -2 & 2 & 1 & -3 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{bmatrix}$$

$R_2 \leftarrow R_2 - R_1$

Gaussian Elimination (Example)

$$\begin{bmatrix} 1 & 0 & -2 & 3 & 5 & -4 \\ 0 & 1 & -2 & 2 & 0 & -7 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{bmatrix}$$

Gaussian Elimination (Example)

next entry to zero

$$\begin{bmatrix} 1 & 0 & -2 & 3 & 5 & -4 \\ 0 & 1 & -2 & 2 & 0 & -7 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{bmatrix}$$

Gaussian Elimination (Example)

next entry
to zero

$$\begin{bmatrix} 1 & 0 & -2 & 3 & 5 & -4 \\ 0 & 1 & -2 & 2 & 0 & -7 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{bmatrix}$$

$R_1 \leftarrow R_1 - 5R_3$

Gaussian Elimination (Example)

$$\begin{bmatrix} 1 & 0 & -2 & 3 & 0 & -24 \\ 0 & 1 & -2 & 2 & 0 & -7 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{bmatrix}$$

Gaussian Elimination (Example)

$$\begin{bmatrix} \boxed{1} & 0 & -2 & 3 & 0 & -24 \\ 0 & \boxed{1} & -2 & 2 & 0 & -7 \\ 0 & 0 & 0 & 0 & \boxed{1} & 4 \end{bmatrix}$$

done with back substitution phase

Question

$$\begin{bmatrix} 1 & 0 & -2 & 3 & 0 & -24 \\ 0 & 1 & -2 & 2 & 0 & -7 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{bmatrix}$$

Write down the general form solution from the given RREF.

Solution

$$\begin{bmatrix} 1 & 0 & -2 & 3 & 0 & -24 \\ 0 & 1 & -2 & 2 & 0 & -7 \\ 0 & 0 & 0 & 0 & 1 & 4 \end{bmatrix}$$

Solution

$x_1 = (-24) + 2x_3 - 3x_4$

$x_2 = (-7) + 2x_3 - 2x_4$

x_3 `is free`

x_4 `is free`

$x_5 = 4$

How-To: Solving a System of Linear Equations

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1. Write your system as an augmented matrix

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2. Find the RREF of that matrix

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1. Write your system as an augmented matrix

2. Find the RREF of that matrix

3. Read off the solution from the RREF

How-To: Solving a System of Linear Equations

1. Write your system as an augmented matrix
2. Find the RREF of that matrix

   Gaussian elimination
3. Read off the solution from the RREF

Numerics

demo

(mini-GE)

Significant Figures (Sig Figs)

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Have you ever been docked points in a science class for having incorrect sig figs?

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when you use a ruler, you can't do better than ± 1mm, so we can't say anything about nanometer differences

Significant Figures (Sig Figs)

Have you ever been docked points in a science class for having incorrect sig figs?

when you use a ruler, you can't do better than ± 1mm, so we can't say anything about nanometer differences

we run into a similar problem with decimal numbers in programs

Number Representations

Number Representations

```
your computer is a collection of fixed size
registers
```

Number Representations

```
your computer is a collection of fixed size
registers

each register holds a sequence of bits
```

Number Representations

your computer is a collection of fixed size registers

each register holds a sequence of bits

The Goal. represent numbers so they fit in those registers

Number Representations

your computer is a collection of fixed size registers

each register holds a sequence of bits

The Goal. represent numbers so they fit in those registers

this is, of course, ~~a lie~~ an abstraction

Number Representations

0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Number Representations

0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Question. How do we slice up our fixed sequence to represent numbers?

Number Representations

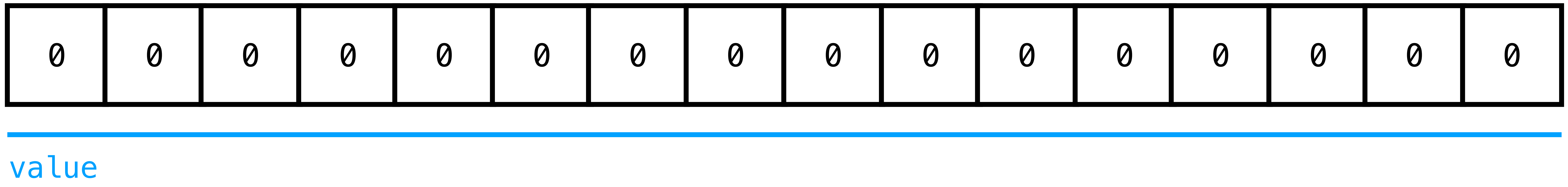
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Question. How do we slice up our fixed sequence to represent numbers?

<u>things to consider:</u>

- simple idea (easy to understand)
- maximize coverage (not too redundant)
- simple numeric operations (easy to use)

Unsigned Integers

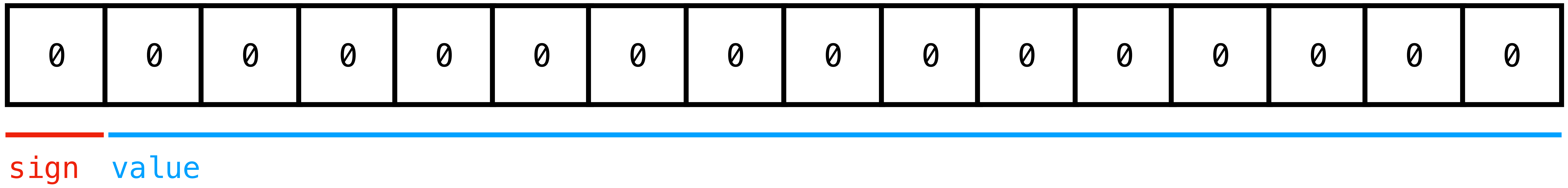


binary value (we should know this by now)

e.g. 10001010 represents

$$1(2^7) + 0(2^6) + 0(2^5) + 0(2^4) + 0(2^3) + 1(2^2) + 0(2^1) + 1(2^0)$$

Signed Integers



`sign bit + binary value`

`e.g. 10001010 represents`

$$-1 \times \left(0(2^6) + 0(2^5) + 0(2^4) + 0(2^3) + 1(2^2) + 0(2^1) + 1(2^0)\right)$$

Floating-Point Numbers (Some Figures)

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`floats in python use 64 bits`

Floating-Point Numbers (Some Figures)

floats in python use 64 bits

That's 1.8×10^{19} possible values

Floating-Point Numbers (Some Figures)

`floats in python use` <u>`64 bits`</u>

`That's` 1.8×10^{19} `possible values`

`We can't represent everything. We'll have to choose and then round`

Floating-Point Numbers (Some Figures)

floats in python use 64 bits

That's 1.8×10^{19} possible values

We can't represent everything. We'll have to choose and then round

Question. Which ones should we represent?

Floating-Point Numbers (An Idea)

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Integers work because they are **discrete and evenly spaced**

Floating-Point Numbers (An Idea)

Integers work because they are **discrete and evenly spaced**

What if we evenly discretize a range of values?

Floating-Point Numbers (An Idea)

Integers work because they are **discrete and evenly spaced**

What if we evenly discretize a range of values?

i.e., represent

..., –0.001, 0, 0.0001, 0.002, 0.003, 0.004,...

Question

Discuss the advantages and disadvantages of this approach

Floating-Point Numbers (IEEE-754)

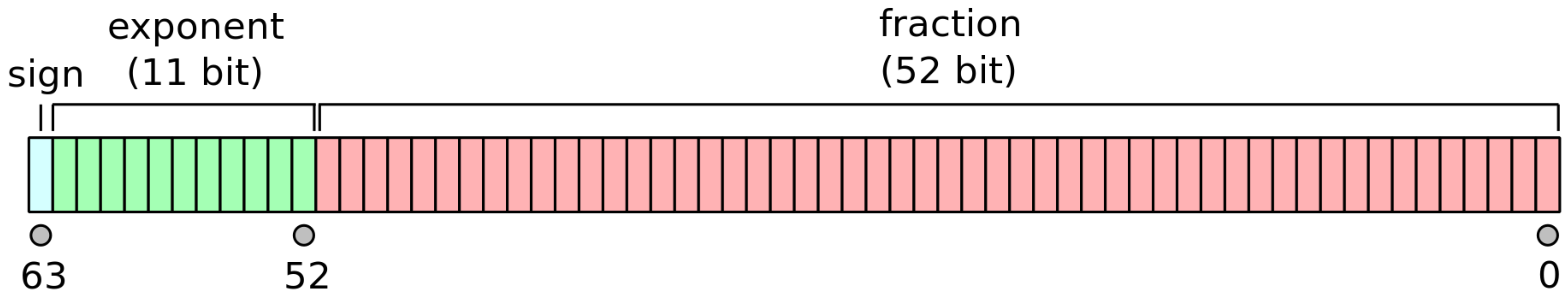
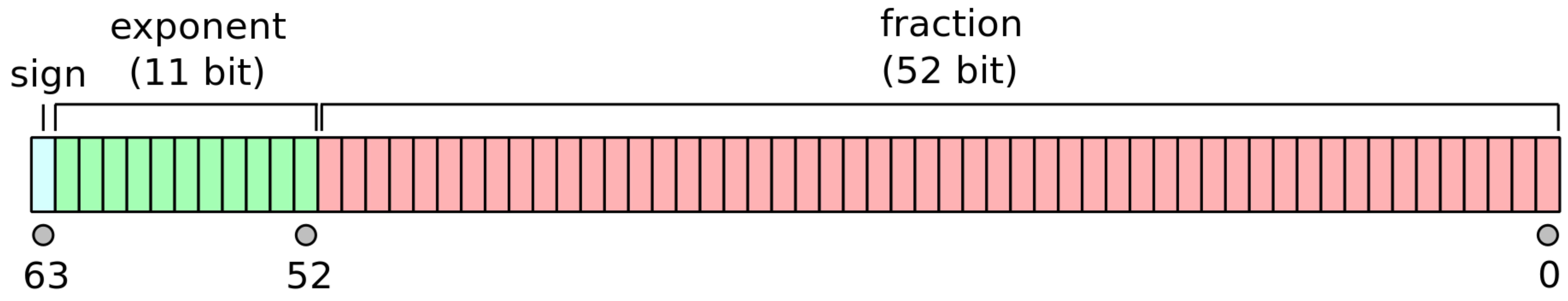


image source

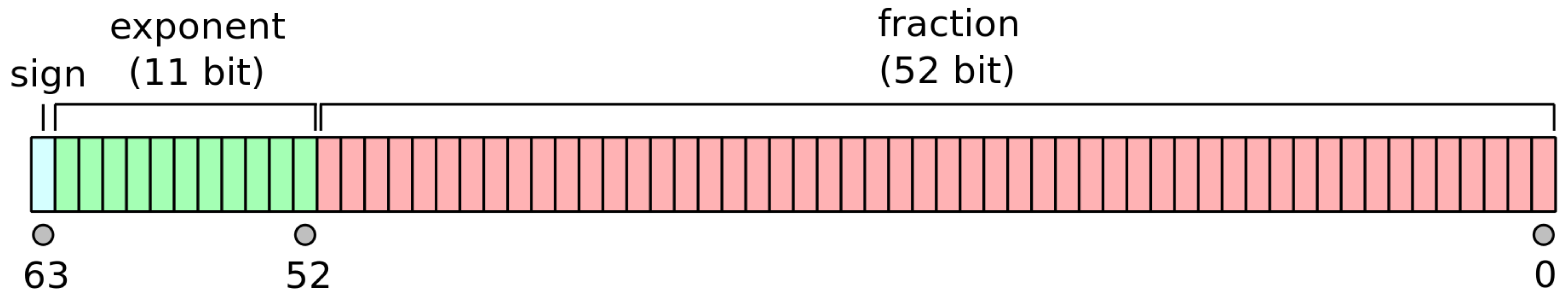
Floating-Point Numbers (IEEE-754)



```
like scientific notation, but binary
```

image source

Floating-Point Numbers (IEEE-754)



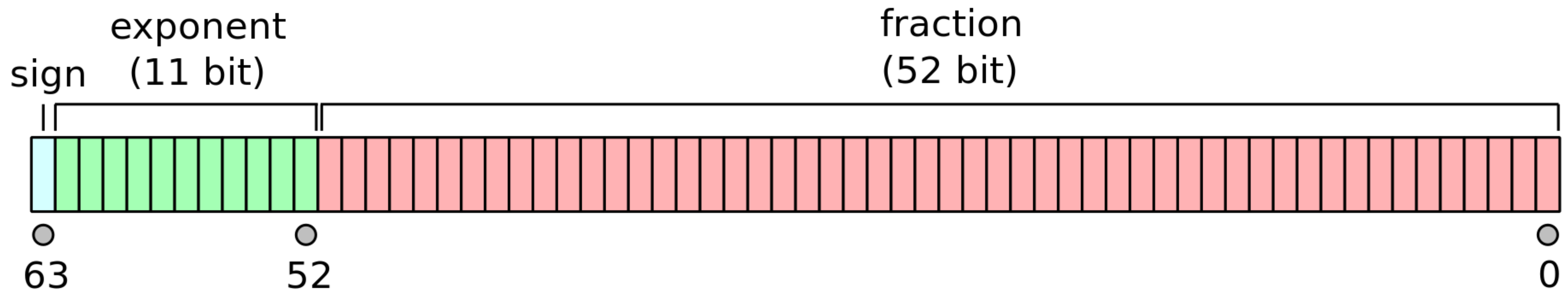
like scientific notation, but binary

the equation:

$$(-1)^{\text{sign}} \times \left(1 + \frac{\text{fraction}}{2^{52}}\right) \times 2^{\text{exponent} - (2^{10} - 1)}$$

image source

Floating-Point Numbers (IEEE-754)



like scientific notation, but binary

<u>the equation:</u>

$$(-1)^{\text{sign}} \times \left(1 + \frac{\text{fraction}}{2^{52}}\right) \times 2^{\text{exponent}-(2^{10}-1)}$$

it's an accepted standard, not perfect, but it works well

image source

Question

$$(-1)^{\text{sign}} \times \left(1 + \frac{\text{fraction}}{2^{52}}\right) \times 2^{\text{exponent}-(2^{10}-1)}$$

Any ideas why this is better/worse?

And why not have a sign bit for the exponent?

Step Size

$$(-1)^{\text{sign}} \times \left(1 + \frac{\text{fraction}}{2^{52}}\right) \times 2^{\text{exponent}-(2^{10}-1)}$$

image source

Step Size

$$(-1)^{\text{sign}} \times \left(1 + \frac{\text{fraction}}{2^{52}}\right) \times 2^{\text{exponent}-(2^{10}-1)}$$

$\longleftarrow$ step size increases with magnitude $\longrightarrow$

Definition. step size is the space between two floating-point representations

image source

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for fixed exponent n two numbers are at least

$$0.00\ldots001 \times 2^n = 2^{-52} \times 2^n$$

away (why?)

image source

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away (why?)

Step size doubles for each exponent

image source

Things to Keep in Mind

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IEEE–754 defines a subset of decimal numbers

operations on floating point numbers attempt to give you the closest to the actual value, though there will be errors.

we can assume when we write down a number like '0.3' we get the closest IEEE–754 value

Relative Error

Observation. ± 0.001 is *tiny* error for 10^{20} but *massive* for 10^{-20}

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IEEE-754 keeps relative error <u>small</u>

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Relative Error (Calculation)

`(fix an exponent` n`)`

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$$(-1)^{\mathsf{sign}} \times \left(1 + \frac{\mathsf{fraction}}{2^{52}}\right) \times 2^{\mathsf{exponent} - (2^{10}-1)}$$

(fix an exponent n)

error is determined by step-size

$$\mathsf{err} \leq 2^{-52} \times 2^{n}$$

$$(-1)^{\text{sign}} \times \left(1 + \frac{\text{fraction}}{2^{52}}\right) \times 2^{\text{exponent}-(2^{10}-1)}$$

Relative Error (Calculation)

(fix an exponent n)

the smallest number we can represent at least 1.0×2^n

$$\text{val} \geq 1.0 \times 2^n$$

(why do we care about a lower bound on val?)

Relative Error (Calculation)

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$\approx$16 digits of accuracy

Not bad, but also not great

demo

(example from the notes)

The Takeaways

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```
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What do we do about it?

Best Practices

1. don't compare floating points for equality
2. be aware of ill-conditioned problems
3. be aware of small differences

Principle 1: Closeness

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When doing floating-point calculations in a program, define an error margin and use that for equality checking

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When doing floating-point calculations in a program, define an error margin and use that for equality checking

In Practice.

```
    Replace    x == y
    with       numpy.isclose(x, y)
```

demo

Principle 2: Ill-Conditioned Problems

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Make sure your problem is not sensitive to small errors.

Principle 2: Ill-Conditioned Problems

Make sure your problem is not sensitive to small errors.

In Practice. for example, don't divide by numbers much smaller than your error tolerance

demo

Principle 3: Small Differences

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Make sure you understand your error tolerance when looking that the small differences of large numbers.

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In Practice. Don't expect $a - b$ to be small when a and b are "close" but very large.

demo

One Last Note: Special Numbers

`0`	`(we can't already represent 0?)`
`nan`	`stands for not a number, .e.g, sqrt(-2)`
`inf`	`symbolic infinity, behaves as expected`

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We will primarily be using numpy (and scipy) instead of sympy in this course.

NumPy vs. Sympy

NumPy is **fast**

NumPy is **approximate**

NumPy is **widely used in applications**

Sympy is **slow**

Sympy is **exact**

Sympy is a **teaching tool** (and useful in symbolic computation research)

NumPy vs. Sympy

`numpy.array(...)`	`Matrix(...)`
`a[i] #row access`	`a[i,:] #row access`
`a[:,j] #col access`	`a[:,j] #col access`
`a.shape[0]`	`a.rows`
`a.shape[1]`	`a.cols`

demo

Extra Topic:
Analyzing Gaussian Elimination

Analyzing the Algorithm

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`We will not use` $O(\cdot)$ `notation!`

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>> addition
>> subtraction
>> multiplication
>> division
>> square root

Analyzing the Algorithm

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>> square root

$2n$ vs. n is very different when $n \sim 10^{20}$

Dominant Terms

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A function $f(n)$ is ***asymptotically equivalent*** to $g(n)$ if

$$\lim_{i \to \infty} \frac{f(i)}{g(i)} = 1$$

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A function $f(n)$ is ***asymptotically equivalent*** to $g(n)$ if

$$\lim_{i \to \infty} \frac{f(i)}{g(i)} = 1$$

for polynomials, they are equivalent to their dominant term

Dominant Terms

the dominant term of a polynomial is the monomial with the highest degree

$$\lim_{i \to \infty} \frac{3x^3 + 100000x^2}{3x^3} = 1$$

$3x^3$ dominates the function even though the coefficient for x^2 is so large

Parameters

n : number of variables

m : number of equations (we will assume $m = n$)

$n + 1$: number of rows in the augmented matrix

The Cost of a Row Operation

$$R_i \leftarrow R_i + aR_j$$

$n+1$ multiplications for the scaling

$n+1$ additions for the row additions

Tally: $2(n+1)$ FLOPS

Cost of First Iteration of Elimination

$$\begin{aligned} R_2 &\leftarrow R_2 + a_2 R_1 \\ R_3 &\leftarrow R_3 + a_3 R_1 \\ &\vdots \\ R_n &\leftarrow R_n + a_n R_1 \end{aligned}$$

`repeated row operations for each row except the first`

`Tally:` $\approx 2n(n+1)$ `FLOPS`

Rough Cost of Elimination

repeating this last process at most n times gives us a dominant term $2n^3$

we can give a better estimation...

Tally: $\approx 2n^2(n+1)$ FLOPS

Cost of Elimination

$$\begin{bmatrix} 0 & \blacksquare & * & * & * & * & * & * & * & * \\ 0 & 0 & 0 & \blacksquare & * & * & * & * & * & * \\ 0 & 0 & 0 & 0 & * & * & * & * & * & * \\ 0 & 0 & 0 & 0 & * & * & * & * & * & * \\ 0 & 0 & 0 & 0 & * & * & * & * & * & * \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

At iteration i, we're only interested in rows after i

And to the right of column i

Cost of Elimination

```
Iteration 1: $2n(n+1)$
Iteraiton 2: $2(n-1)n$
Iteration 3: $2(n-2)(n-1)$
     ⋮                      +
```

$$\sum_{k=1}^{n} 2k(k+1) \approx \frac{2n(n+1)(2n+1)}{6} \sim (2/3)n^3$$

Tally: $\sim (2/3)n^3$ FLOPS

Cost of Back Substitution

```
(Let's assume no free variables)

for each pivot, we only need to:

  >> zero out a position in 1 row (0 FLOPS)
  >> add a value to the last row (1 FLOP)
```

at most 1 FLOP per row per pivot $\sim n^2$

Tally: $\sim (2/3)n^3$ FLOPS

Cost of Gaussian Elimination

Tally: $\sim (2/3)n^3$ FLOPS

(dominated by elimination)

Summary

floating point numbers are represented in your computer

floating point operations are not exact

this can have unintended consequences

we get 16 digits of accuracy