Writing, Programming, and Proof

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Context

- Teaching *Computational Mathematics* is increasingly important (Data Science, Visualization, Machine Learning, . . .)
- This is *difficult* because computational mathematics involves several things at once: mathematics, programming, complexity, and numerical stability, because of the *compromises* needed for efficiency.
- The chief compromise (for memory efficiency) is to use *floating-point* arithmetic instead of exact arithmetic.

Why not compute exactly?

Consider the simple question of solving the following linear system of equations.

$$\begin{bmatrix} -81 & -98 & -76 & -4 & 29 \\ -38 & -77 & -72 & 27 & 44 \\ -18 & 57 & -2 & 8 & 92 \\ 87 & 27 & -32 & 69 & -31 \\ 33 & -93 & -74 & 99 & 67 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

The students are taught in their first course to find the *inverse*. [We try to cure them of this.] For this five by five matrix, Maple or other computer algebra systems work fine.

The inverse

$$A^{-1} = \begin{bmatrix} -\frac{5396765}{31934714} & \frac{7836137}{31934714} & -\frac{541124}{15967357} & -\frac{813681}{31934714} & -\frac{850307}{15967357} \\ \frac{3136013}{79836785} & -\frac{851997}{15967357} & \frac{1144771}{79836785} & \frac{1144922}{79836785} & \frac{398039}{79836785} \\ \frac{6211662}{79836785} & -\frac{2183568}{15967357} & \frac{1004049}{79836785} & \frac{77321}{159673570} & \frac{6240977}{159673570} \\ \frac{2291472}{11405255} & -\frac{695571}{2281051} & \frac{449899}{11405255} & \frac{384233}{11405255} & \frac{852141}{11405255} \\ -\frac{11684919}{159673570} & \frac{3340737}{31934714} & -\frac{622854}{79836785} & -\frac{2680781}{159673570} & -\frac{1529291}{79836785} \end{bmatrix}$$

However, for even such a modest example, *the answer is nearly unintelligible*, and the *memory usage during the computation is nearly unpredictable*.

So we use IEEE floats instead

- IEEE 754/854 Floating-Point Standard means portable code
- Predictable memory usage implies *efficiency*
- Thousands of times faster

Challenges from IEEE floats

- "Admit, for instance, the existence of a minimum magnitude, and you will find that the minimum which you have introduced, small as it is, causes the greatest truths of mathematics to totter." — Aristotle
- Floats are *not associative*: $a + (b + c) \neq (a + b) + c$ necessarily. For instance $-M + (M + 1) = 0$ while $(-M + M) + 1 = 1$ if $M = 3.14 \cdot 10^{17}$.
- This (and other features) break students' models of how the world works.
- **Needs special algorithms** e.g. **QR** algorithm for eigenvalues

A Challenging Example

Consider matrices of the form

$$\begin{bmatrix} 0 & U_1 & 0 & 0 & 0 & 0 & 0 \\ -U_1 & 0 & U_2 & 0 & 0 & 0 & 0 \\ 0 & -U_2 & 0 & U_3 & 0 & 0 & 0 \\ 0 & 0 & -U_3 & 0 & U_4 & 0 & 0 \\ 0 & 0 & 0 & -U_4 & 0 & U_5 & 0 \\ 0 & 0 & 0 & 0 & -U_5 & 0 & U_6 \\ 0 & 0 & 0 & 0 & 0 & -U_6 & 0 \end{bmatrix}$$

where each U_i can be one of $\{1, i, 1+i, 1-i\}$ (here $i^2 = -1$). Thus there are exactly $4^6 = 4096$ such matrices. We will compute all of the eigenvalues of all of these matrices and plot them all on the same graph.

Eigenvalue Pictures (Maple)

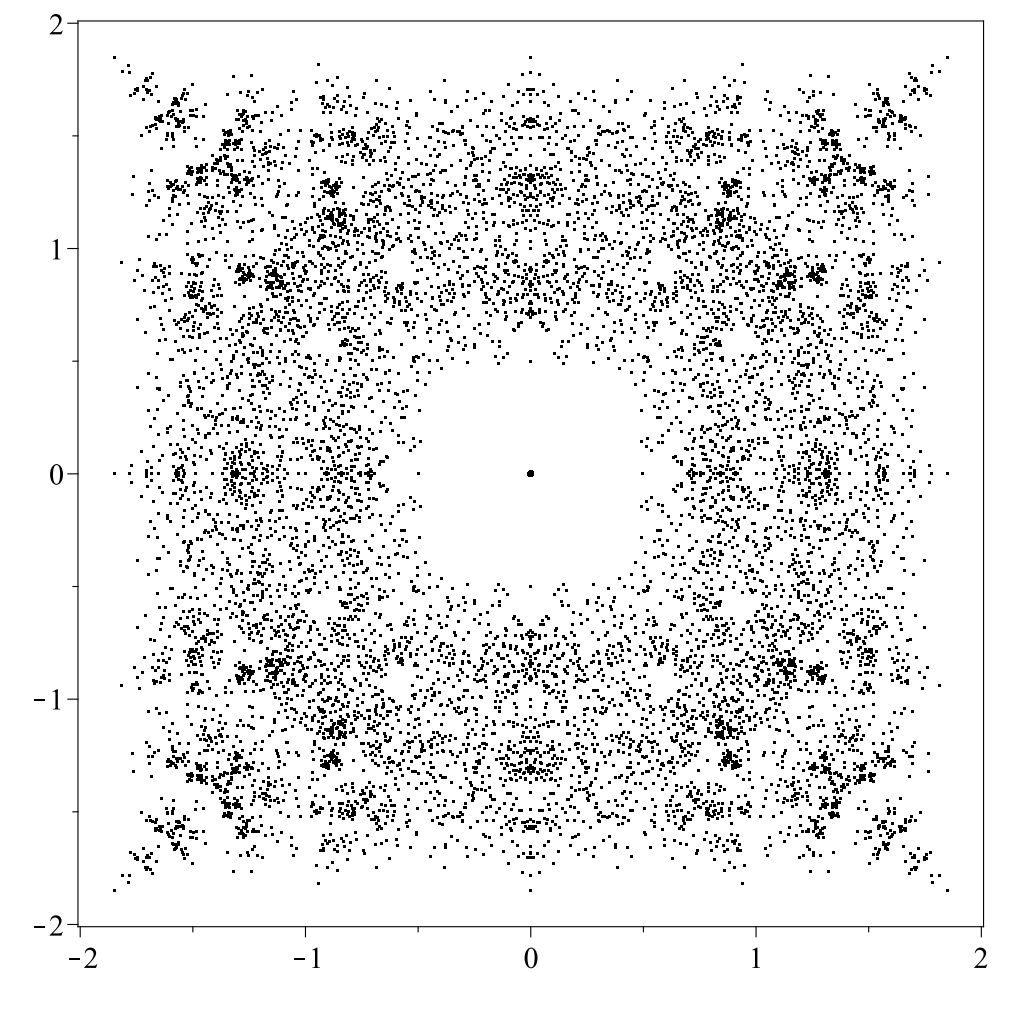


Figure 1: All eigenvalues computed numerically by Maple of all 4096 seven by seven skew-symmetric bidiagonal matrices with entries from $\{1, i, 1+i, 1-i\}$.

Zooming In

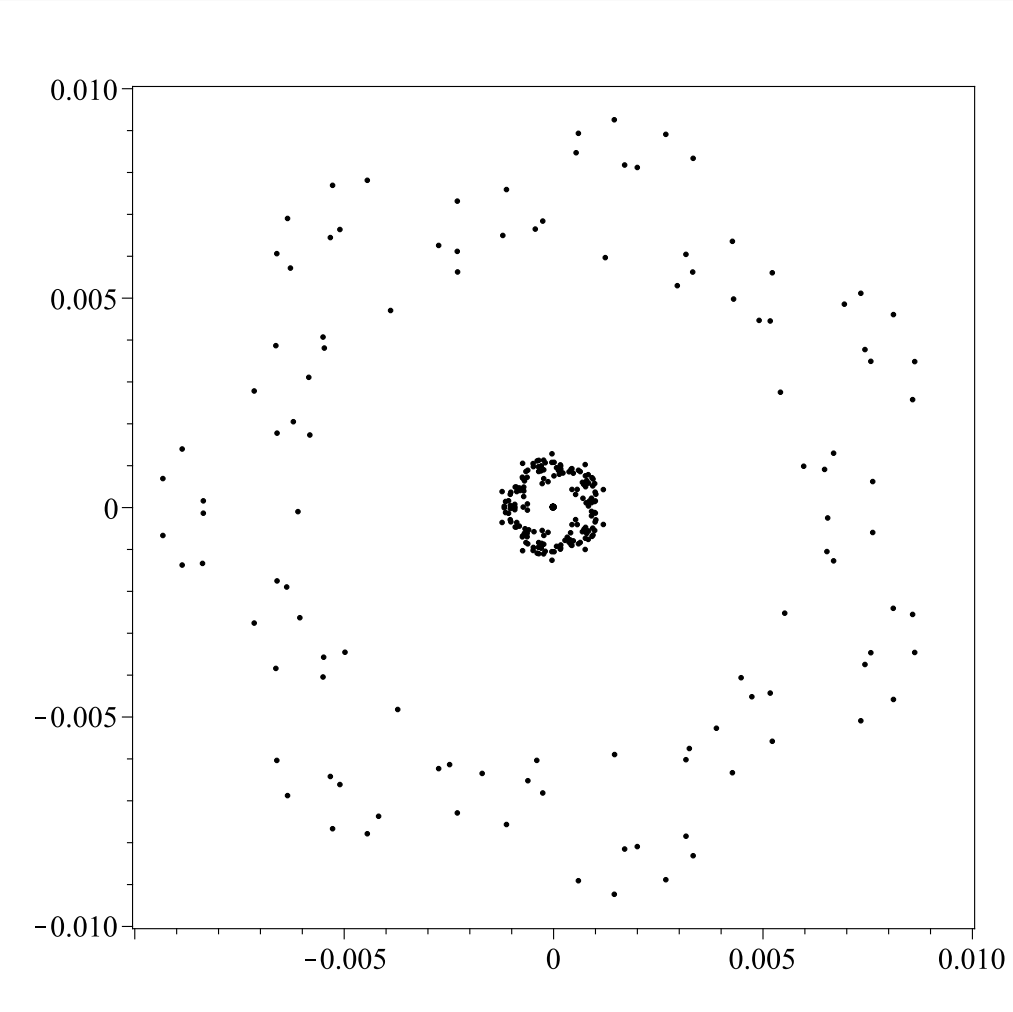


Figure 2: Zooming in on eigenvalues computed numerically by Maple of all 4096 seven by seven skew-symmetric bidiagonal matrices with entries from $\{1, i, 1+i, 1-i\}$.

Zooming In More

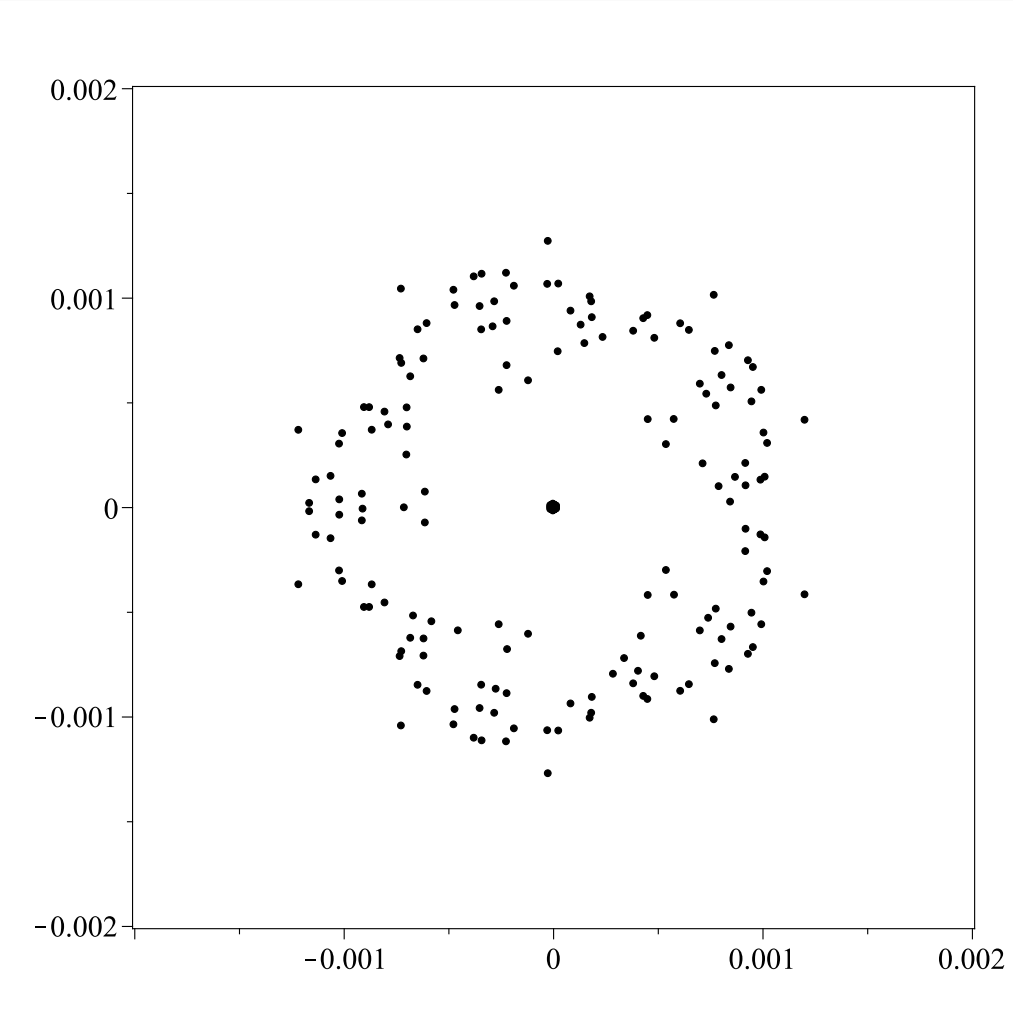


Figure 3: Zooming in more on eigenvalues computed numerically by Maple of all 4096 seven by seven skew-symmetric bidiagonal matrices with entries from $\{1, i, 1+i, 1-i\}$.

Zooming In Even More

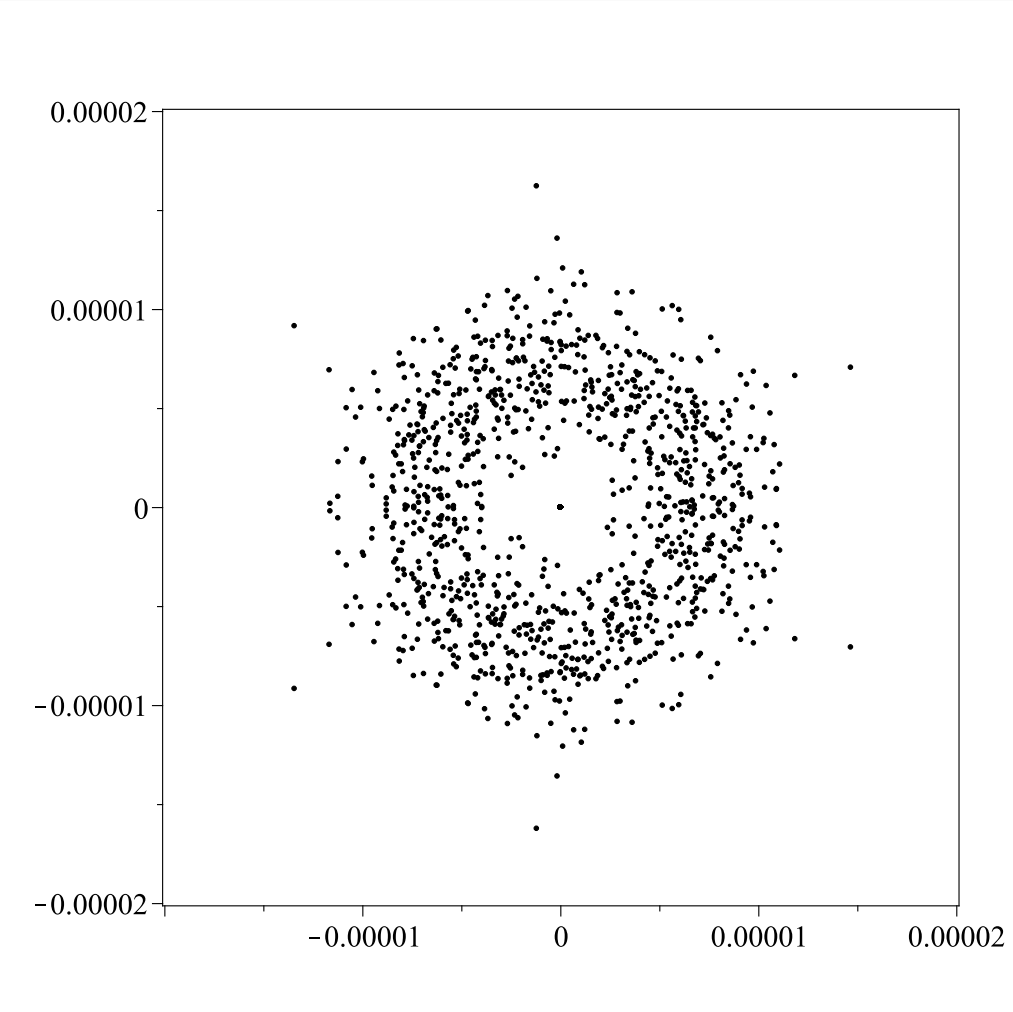


Figure 4: Zooming in even more on eigenvalues computed numerically by Maple of all 4096 seven by seven skew-symmetric bidiagonal matrices with entries from $\{1, i, 1+i, 1-i\}$.

Are they right?

- When we compare the results to those done in Matlab, they seem *exactly the same*.
- The eigenvalues have a *pleasing symmetry*: seven-fold at the 0.01 scale, five-fold at the 0.001 scale, and three-fold at the 10^{-5} scale.

Are they right? [symbolic check with Maple and its CodeGeneration[Matlab]]
http://publish.uwo.ca/∼rcorless/Maple2019/

These small eigenvalues are Rounding Errors

- One can prove mathematically that the eigenvalues of this set of matrices has D_4 symmetry. This means that all these small eigenvalues with non-D_4 symmetry must really be 0.
- **It is a great surprise to students that rounding errors are not random.** Such surprises are didactically useful.
- The seven-symmetric roots come from matrices with λ^7 as their characteristic polynomials; the five-fold from matrices with a factor λ^5; the three-fold from matrices with a factor of λ^3. Multiple roots are infinitely ill-conditioned.
- Roots of $\lambda^7 = 10^{-14}$ are symmetric about 0 and of magnitude 0.01. “Exact eigenvalues of nearby matrices”

Upsetting the Quadratic Formula

Solve $x^2 - 2bx + 1 = 0$ for many large values of b using the quadratic formula: $x_{1,2} = b \pm \sqrt{b^2 - 1}$. The product of these roots is $b^2 - (b^2 - 1) = 1$. **But the quadratic formula is unstable.**

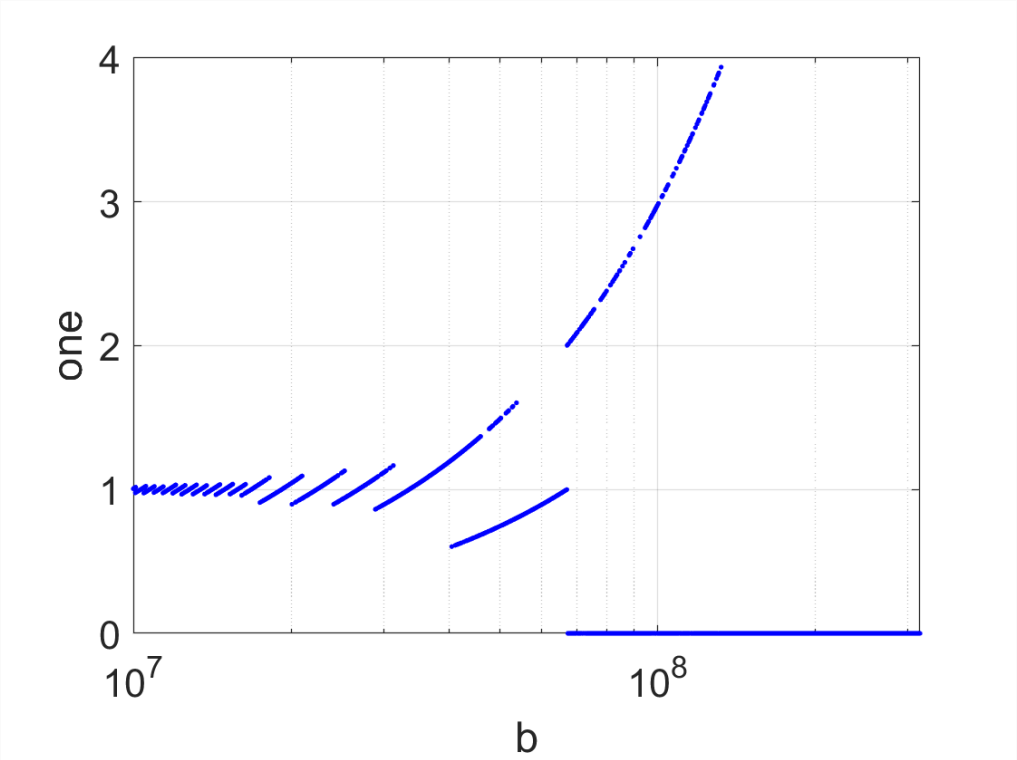


Figure 5: The product of two computed (unstable) quadratic formula roots, for different values of the parameter b.

The importance of Backward Error

- The students must learn to *reverse their perspective*. (Painful, but necessary)
- One useful tool for this is that a **numerically stable** algorithm gives (nearly) **the exact answer to a nearby question**.
- We use this uniformly on all topics: polynomial evaluation, rootfinding, solving linear systems, solving differential equations, etc.
- The students also need to learn that *some problems are sensitive to changes* or **ill-conditioned**.

Principles of Scientific Programming

- The Programmer is Responsible for the Result
- The Modeller should know what is going on in the program
- The Person Should be Able to Explain (and Reproduce) the Result

Principles of Numerical Analysis

- A good numerical method gives (nearly) the exact solution to nearly the right problem
- Some problems are sensitive to changes in their data or models.

The role of writing

"Good writing is clear thinking made visible."—Ambrose Bierce

1. Promotes precision
2. Enhances error-checking
3. A good essay is like a good program is like a good proof:
    - 3.1 defines its terms
    - 3.2 includes enough detail for a person "skilled in the art" to fill in the rest
    - 3.3 makes its conclusions clear

Forcing students to *create a narrative* forces them to think about what the results *mean*, not just what they *are*.

An example problem

Campus Circus

Your TA, Eunice Chan, also works as a part-time stunt performer. She is planning on being catapulted from the entrance of Middlesex college to the main doors of University Hospital, a distance of 605m. A 55kg undergraduate student is catapulted first to test the catapult to make sure Eunice will land close to the hospital.

Measurements of the speed resolved into x and y coordinates are taken from the undergraduate student's smartwatch. The file `speed2018.mat`, which can be downloaded from OWL, contains the speed data. To load this data into MATLAB use the following command

```
load speed2018.mat
```

This loads three variables:

- `t` The time points at which the measurements were taken, in seconds.
- `speedx` The speed in the x direction, in $\frac{\text{m}}{\text{s}}$
- `speedy` The speed in the y direction, in $\frac{\text{m}}{\text{s}}$

Figure 6: Example of lab problem from the quadrature unit for our course AM 2814 (Numerical Analysis)

An example problem

Table 1: Table of variables provided by *speed2018.mat* data file

index	1	2	···	39	40
t	0	0.2769	···	10.5231	10.8000
speedx	64.1547	63.1874	···	52.0130	47.0933
speedy	55.6829	55.3540	···	−52.8820	−53.8300

An example problem

- Numerically integrate the speed data in each direction using the Trapezoid rule to get the distance in each direction. That is compute

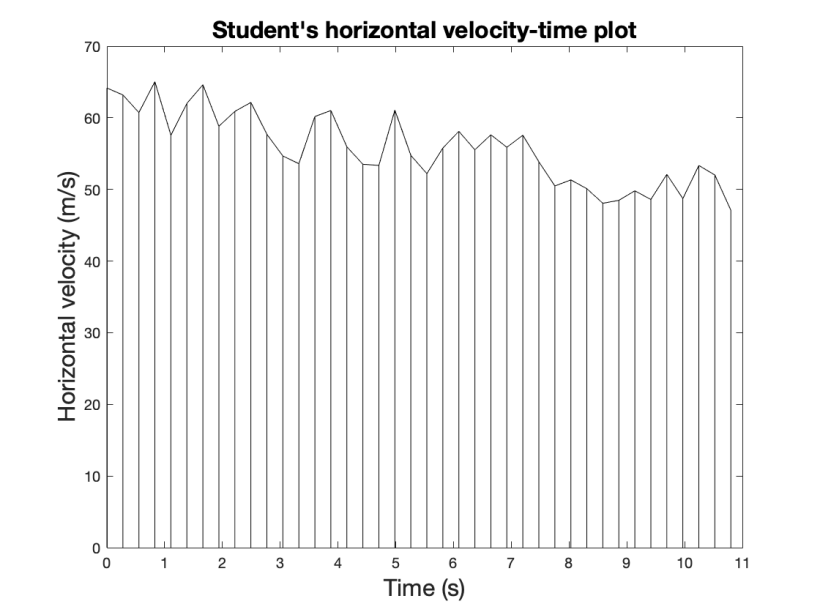
$$d_x(t_i) = \int_{t=0}^{t_i} v_x(t)\,\mathrm{d}t$$
$$d_y(t_i) = \int_{t=0}^{t_i} v_y(t)\,\mathrm{d}t$$

  where $d_x(t)$ is the distance in the x direction at time t and $d_y(t)$ is the distance in the y direction. You must compute this for all values of i. (Note: you will need to write a `trapezoidRule` function that works with vector input). You can use the built-in trapezoid rule function `trapz` in MATLAB if you would like.

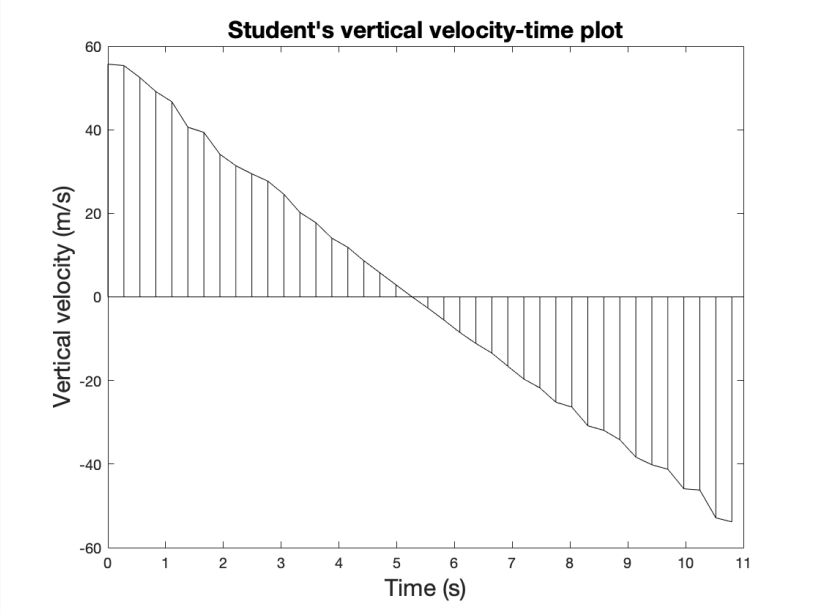
- Make a plot of the trajectory of the undergraduate student (i.e. $d_y(t)$ versus $d_x(t)$)
- Based on your analysis, does the undergraduate student land close to the hospital entrance (within 10m). What is the total distance travelled in the x direction?

Figure 7: Second part of the example of lab problem from the quadrature unit for our course AM 2814 (Numerical Analysis)

An example problem



(a) Horizontal velocity-time plot



(b) Vertical velocity-time plot

Figure 8: Velocity-time plots for example problem

An example problem

```
function T = vecTrapz(v, t)
    if (length(v) ~= length(t))
        error(["The lengths of the vectors"...
        "should be the same."]);
    end
    n = length(v);
    h = t(2) - t(1);
    T = 0;
    for i = 1:(n-1)
        T = T + ((v(i) + v(i+1))/2)*h;
    end
end
```

An example problem

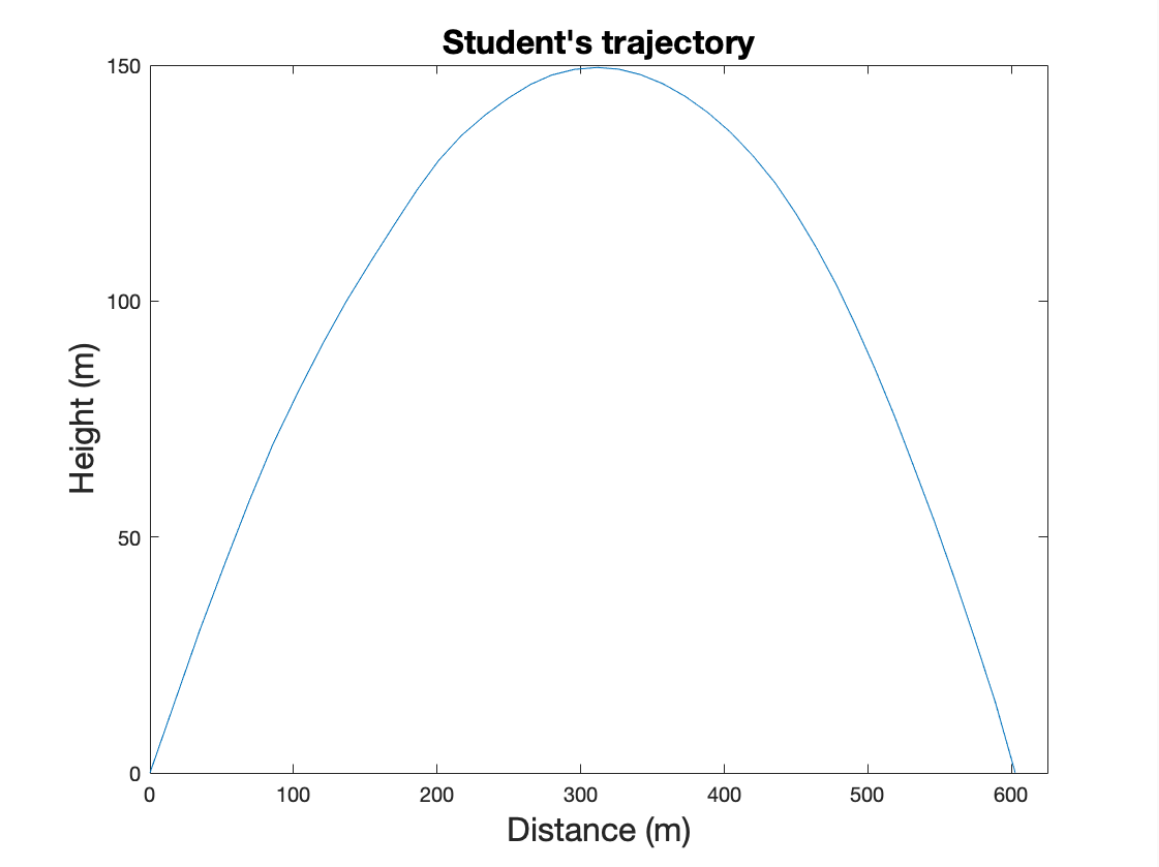
```
load speed2018.mat

dx = zeros(size(t));
dy = zeros(size(t));

for i = 2:length(t)
    dx(i) = vecTrapz(speedx(1:i), t(1:i));
    dy(i) = vecTrapz(speedy(1:i), t(1:i));
end

plot(dx, dy);
axis([0, 625, 0, 150])
xlabel('Distance (m)')
ylabel('Height (m)')
title("Student's trajectory")
```

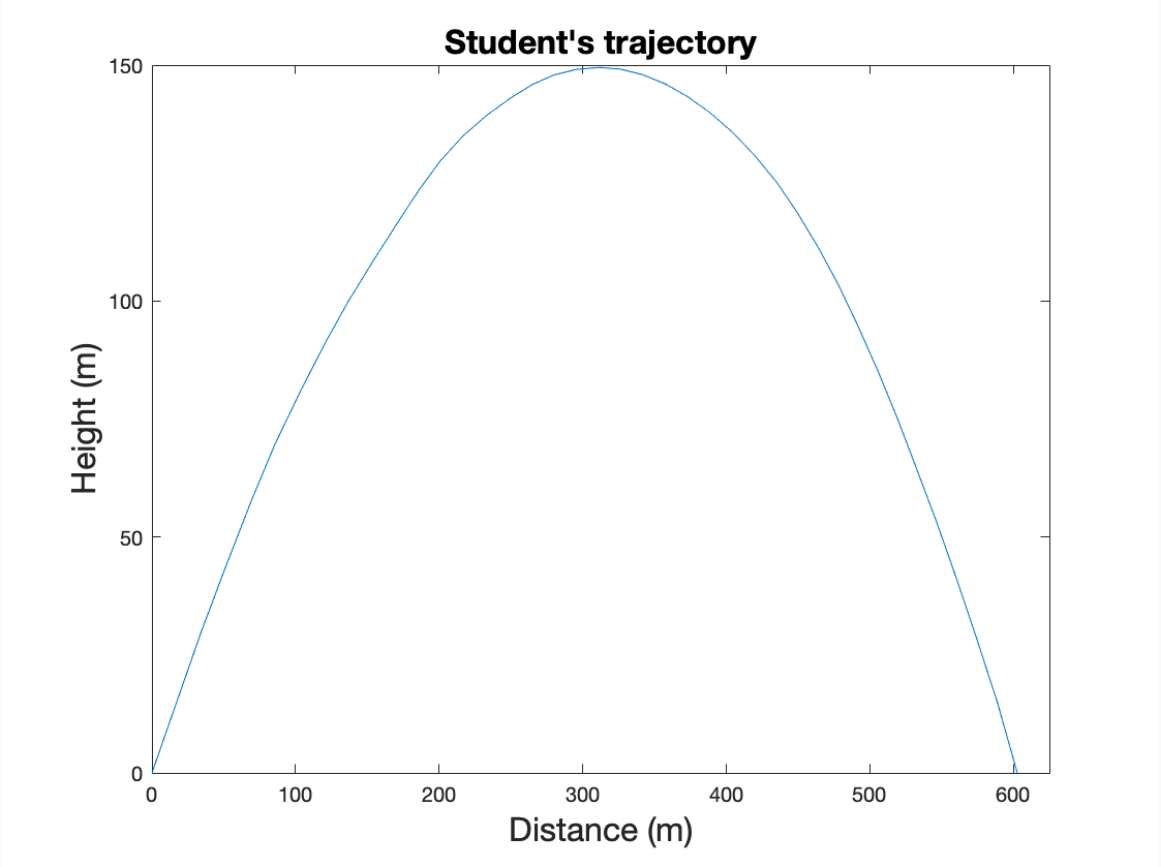
An example problem



(a) Solution to the example problem

Figure 9: Solution to example problem

An example problem



(a) Solution to the example problem

```
>> max(dy)

ans =

   149.5001

>> dx(end)

ans =

   602.5728
```

(b) Maximum height and horizontal distance

Figure 9: Solution to example problem

Reference Papers

Chauvenet prize-winning papers

1. The Perfidious Polynomial — J. H. Wilkinson
2. The Simple Continued fraction for e — C. D. Olds
3. Leonhard Euler's Integral — Philip J. Davis

Reference Texts and Videos

1. Numerical Computing with Matlab — Cleve Moler
2. Matlab Guide — Des Higham and Nick Higham
3. The Elements of Matlab Style — Richard K. Johnson
4. MIT OpenCourseWare: Gil Strang and Cleve Moler

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Thank You

¡Time for Questions!