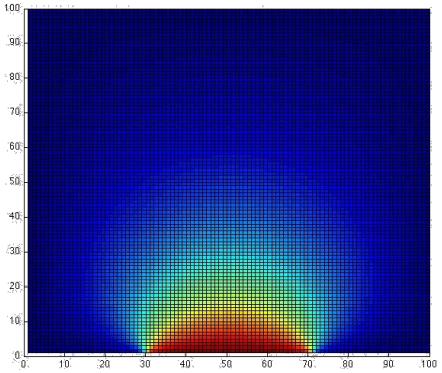


Lecture 01:

Welcome to CS 111

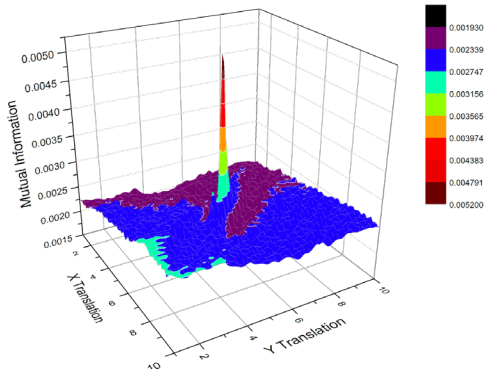
"Introduction to Computational Science"

CS 111: Intro to Computational Science

Spring 2023

Ziad Matni, Ph.D.

Dept. of Computer Science, UCSB



$$\frac{\partial \sigma_{rr}}{\partial r} + \frac{1}{r}\frac{\partial \sigma_{r\theta}}{\partial \theta} + \frac{\partial \sigma_{rz}}{\partial z} + \frac{1}{r}(\sigma_{rr} - \sigma_{\theta\theta}) + F_r = \rho \frac{\partial^2 u_r}{\partial t^2}$$

$$\frac{\partial \sigma_{r\theta}}{\partial r} + \frac{1}{r}\frac{\partial \sigma_{\theta\theta}}{\partial \theta} + \frac{\partial \sigma_{\theta z}}{\partial z} + \frac{2}{r}\sigma_{r\theta} + F_\theta = \rho \frac{\partial^2 u_\theta}{\partial t^2}$$

$$\frac{\partial \sigma_{rz}}{\partial r} + \frac{1}{r}\frac{\partial \sigma_{\theta z}}{\partial \theta} + \frac{\partial \sigma_{zz}}{\partial z} + \frac{1}{r}\sigma_{rz} + F_z = \rho \frac{\partial^2 u_z}{\partial t^2}$$

Your Instructor

Ziad Matni, Ph.D.

(zee-ahd mat-knee)

Assistant Teaching Professor in Computer Science

About me…

What to Call Me?? *Prof. Matni!*

Teaching: *CS, Data Science, Computational Social Science*

Research: *CS Education, Information Seeking Behavior, Social Networks*

Other: *CS Advisor to 1st year students and TikTok Influencers* *(no, not really that last thing…)*

The CS 111 Instructional Team

Teaching Assistants (TAs)

Anjie Chen

Zichen Chen

Qiming Wu

Undergrad Learning Assistants (ULAs)

Kirill Aristarkhov

Guang Yang

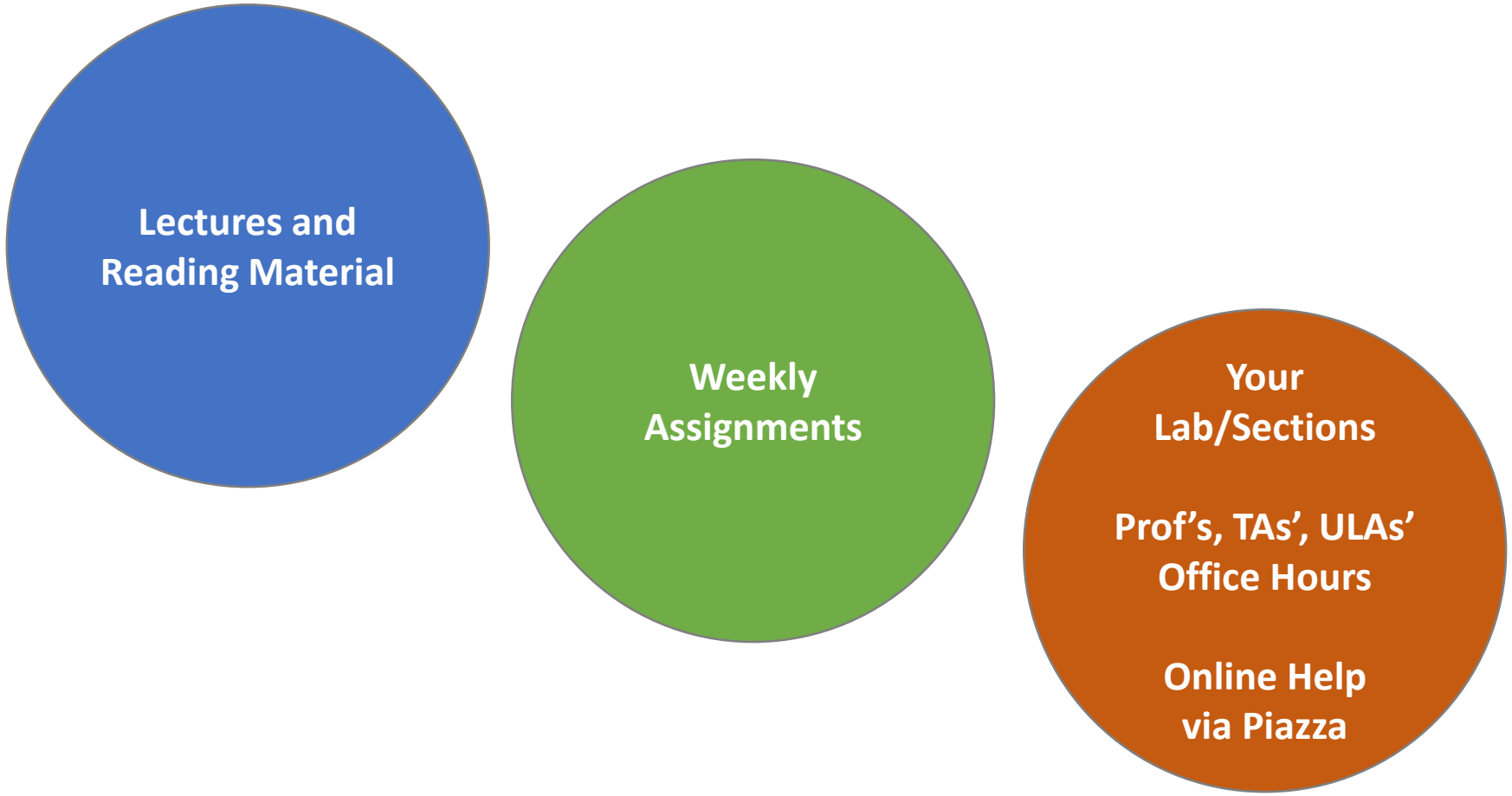
How About You?!

Who are YOU?!?!?!

Also:

1. ***Trying to add the class?***
2. ***Trying to switch labs?***
3. ***Taking attendance***

The Trifecta of Success in this Class!



Where is Everything? What Should I Get?

- You NOW have accounts ready on the following (i.e. I have registered you):
  - Canvas
  - Gradescope
  - Piazza

PLEASE CHECK THAT YOU HAVE ACCESS!!!

- **Software for this course:**
  - Python 3.9+ (recommend: **Jupyter Notebook**)
  - LaTeX editor / PDF creator (recommend: **OverLeaf.com**)
  - More on these in your first lab this week!

Main Class Website…

…will be on **CANVAS**

On there, I will keep:

- Latest syllabus (incl. schedule)
- Class assignments
- Important handouts and articles
- Exam prep material
- Etc…

Lab/Discussion Sections

- T.As will be available for questions about the lab during the lab times
  - **Thursdays 4 PM, 5 PM, and 6 PM – in person!!**
  - Attendance is **taken** (you can skip up to 2 labs w/o penalty)

- We **STRONGLY** **encourage** you to ask the TAs questions to help you understand what you may have missed in lecture or readings.

Quizzes and Exams

- Instead of a midterm, I will have weekly quizzes
  - **Starting NEXT week**
  - All quizzes are taken in the classroom **every Wednesday** at the **start of class**

- Cumulative Final Exam on **Wed. June 14th at 8:00 AM**
  - In person, in this classroom

- NO make up for missed quizzes or exams

Format of Assignments

- Given every Monday
- Discussed in lab on Thursday
- Due by Monday

- This class will have **weekly assignments**
  - Posted online via **Canvas**
  - You will turn them into **Gradescope** by the due date

- Process:
  - I give you a PDF ***and*** a LaTeX source code for it
  - You **edit** the LaTeX source code and insert your answers
  - You **save** your work **as a PDF**
  - You **upload** the PDF onto **Gradescope**

- **Some of the labs will be programs (in Python) to submit on Gradescope**

LaTeX

- A **markup language** used a lot in Engineering & Math
- Makes elegant formats for equations, matrices, code, etc…
- Many free apps out there for this.
  - We recommend **overleaf.com**
- **The 1st Lab will go over LaTeX syntax/use**

```
30 {\bf 1.}
31 A variation of the {\em Kermack-McKendrick model}

32 for the course of an epidemic in a population is
   given by the system of ODEs
33 \begin{align}
34 \dot y_0 &= -cy_0y_1, \\
35 \dot y_1 &= cy_0y_1 - ry_1 - dy_1, \\
36 \dot y_2 &= ry_1, \\
37 \dot y_3 &= dy_1,
38 \end{align}
```

!!

1. A variation of the *Kermack-McKendrick model* for the course of an epidemic in a population is given by the system of ODEs

$$\dot{y}_0 = -cy_0y_1, \tag{1}$$
$$\dot{y}_1 = cy_0y_1 - ry_1 - dy_1, \tag{2}$$
$$\dot{y}_2 = ry_1, \tag{3}$$
$$\dot{y}_3 = dy_1, \tag{4}$$

where y_0 represents susceptibles, y_1 represents infectives in circulation, y_2 represents infectives removed by recovery and immunity, and y_3 represents infectives removed by death. The parameters c, r, and d represent the infection rate, recovery rate, and death rate, respectively.

Use `integrate.solve_ivp()` to solve this system numerically, with the parameter values $c = 1$, $r = 5$, and $d = 1$, and initial values $y_0(0) = 95$, $y_1(0) = 5$, and $y_2(0) = y_3(0) = 0$. Solve for times $t = 0$ to $t = 1$.

Do I HAVE to use LaTeX????

Yes!!

Can I use Something Else???

Google Docs is just as good!

- Not for this class… (for consistency and learning outcomes)
  - You ARE expected to graduate knowing LaTeX and will use it in other courses in CS

- *LaTeX is a very useful tool for Engineers in both academia AND industry.*
  This is a good skill for you to acquire and put on your resumes!

Getting Help from Us

- **Office Hours!**
  - Are listed in syllabus and on Canvas
  - There's the instructor (me!), the TAs (3 of them!) ***and*** the ULAs (2 of them!) to help you out!
- **Piazza!**
  - We will check-in daily to help there
  - Students should help each other out too!!
- **Email!**
  - *But only if you have to*, **e.g. if it's personal**.
  - If you are emailing us, **PLEASE** say it's CS111-related in the subject field

About This Course

- This is an **introductory** course in **Computational Science**
- Methods/algorithms to
  solve various scientific and data problems via cool computations!
- Very useful for future classes in Advanced Data Science and Machine Learning
- Not a theory course per se, but we'll bring it up once in a while

About This Course: What We'll Cover

- Optimizing complex calculations and scientific sims of models that require MATH!

  Linear Algebra, Ordinary and Partial Differential Equations (ODEs + PDEs)

- Methods to make "heavy" computations more efficient through certain techniques, like:

  Fast matrix factorizations (Cholesky, Jacobi, Conjugate Gradient, Q-R)

  Singular Value Decomposition (SVD)

  Principal Component Analysis (PCA)

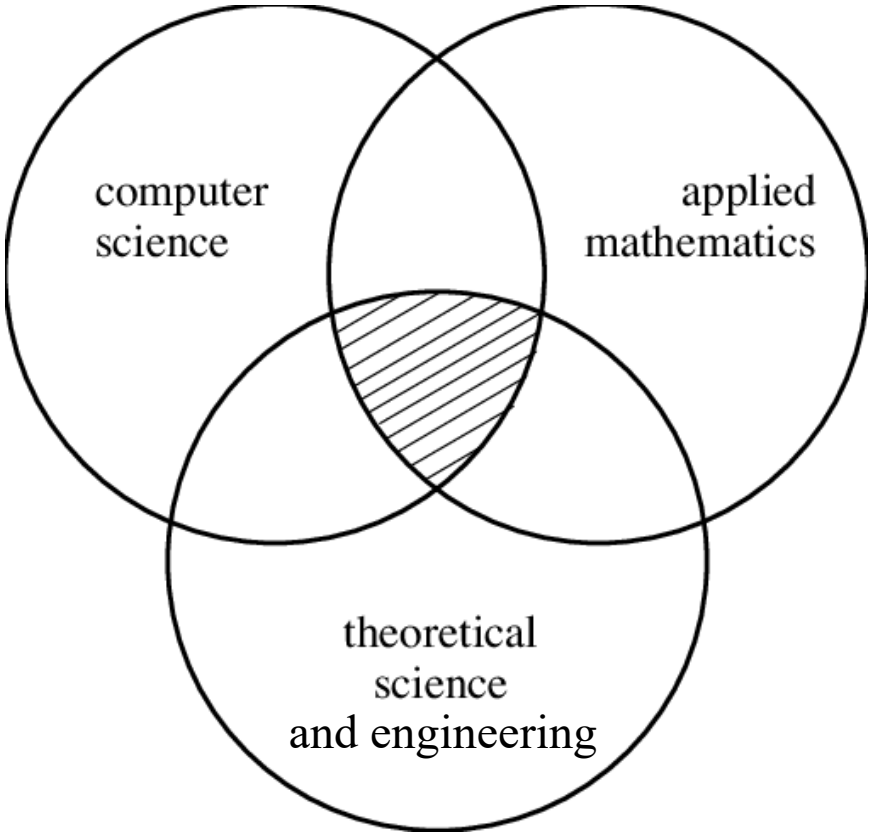
  PageRank and Graphs

About This Course

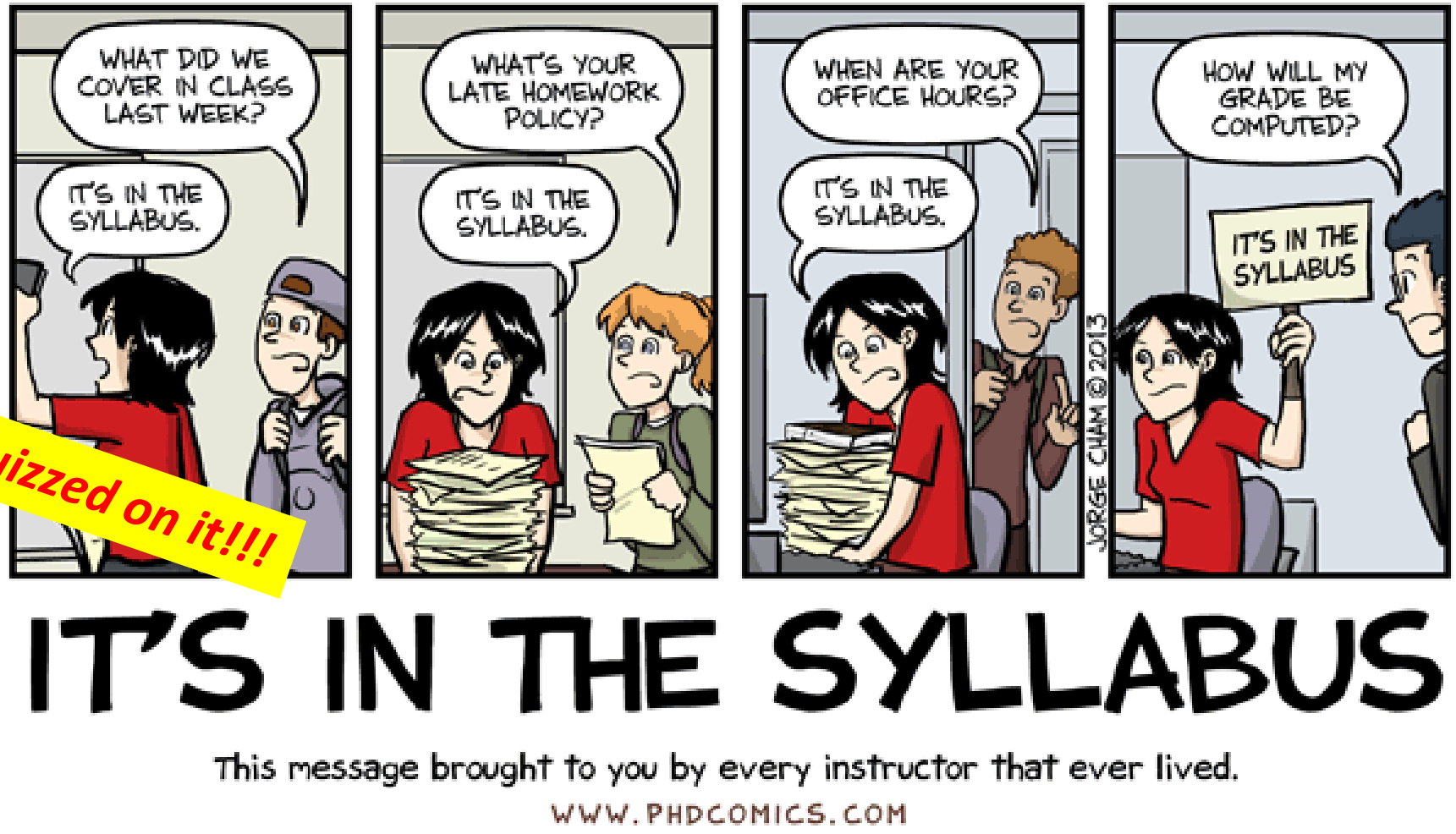
- This course can sometimes be “heavy” on new concepts and on stuff from older Math classes you’ve taken
  - Be SURE you keep up with the **LECTURES**, **READINGS, LABS,** and **OFFICE HOURS**!
- I do expect you to be very comfortable with Linear Algebra (and math, in general)
- I do expect you to get comfortable with the Python language rather quickly
  - Luckily it’s not hard… AND I will give you TONS of examples/demos
  - You SHOULD “**play around**” with the code at home
    - Experimentation is GOOD for learning!!! Making mistakes is GOOD for learning!!!

Applications Of Computational Science

- Data Science
- Applied Math and Statistics
- Modeling Physical Phenomena in Engineering
- Machine Learning Algorithms
- Computational finance
- Computational biology



Just in Case…



You will be quizzed on it!!!

My Policies (Details in Syllabus)

- Grading
  - Assignments: 35% Quizzes: 30% Final: 35%
- Late Policy
  - Assignments turned in after due, within 24 hrs: **Lose 20%**
  - No late assignments accepted after 24 hrs: **zero grade**
- Make-up Policy
  - ***No*** make-ups given on any quizzes or final exam

What Happens in a Typical Week in CS 111?

- MONDAY
  Come to lecture 1
  We release the week's assignment
- WEDNESDAY
  Come to lecture 2
  Take the weekly quiz at the start of class (10-15 mins)
  (again, note: there is NO quiz THIS 1st week…)
- THURSDAY
  Go to lab/section – discussions are *often* about assignments!
- WEEKEND
  Finish your assignment (start early, though!!)
  Assignments are typically due every **Monday by 11:59 PM**
  (on Gradescope)

Textbook?

- This course does not have a textbook
- BUT, I will give you PDF readings that I EXPECT you to do!
- Mostly from
  - *Numerical Computing with Matlab* by Cleve Moler
  - Other sources

Need a Refresher on Linear Algebra Concepts?

- We'll cover some things this week…
- You can also check out **Prof. Gilbert Strang**'s videos from MIT Coursera
  - Link is on Canvas and also in Syllabus
- Review your MATH 4A and MATH 4B class notes, especially for:
  - Matrix multiplication
  - Matrix factorization
  - Eigenvalues and Eigenvectors
  - Solving Ax = b via Gaussian Elimination

Python Crash Course

get to know how to do these basic things…

- Comments (typically use **#**)
- **import** statements
- Basic variable types: **int**, **str**, **float**, **bool** (True/False)
- Other variable types: **list**, **tuples**
- Converting from one data type to another **int("360")** **string(360.77)**
- Standard output/input: **print()** **input()** # prints string; gets input as str
- Importance of *tabbed spaces* (to define a block – instead of { … } like in C++)
- Conditionals: **if a > 5:**
- For-loops **for k in range(10):** **for k in ("cs111"):**
- While loops **while a > 5:**
- Defining Functions **def funcX(m, n):** # you don't need to say if it's a void/int/etc… type of function
- File I/O

Useful Python Modules

We usually `import` these at the start of the program (similar to **#include** in C++)

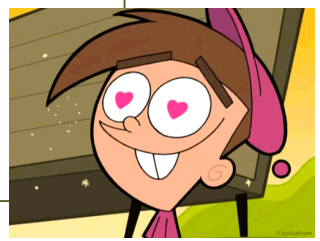
- `math` # common math & trig functions
- `numpy` # fundamental package for scientific computing – We will be using this A LOT!
- `Matplotlib` # plotting package for 2D + 3D plots
- `scipy` # contains the above + other important algos/stats mods

What the !@#* is a LaTeX???

- A very popular *markup* language/system with high-quality *typesetting*
- Used to produce technical and scientific documentation.
- Allows you to consistently produce this sort of output:

$$E_i[\eta_n^k - \eta]^2 \leqslant K_i \frac{1}{\left|T_k\left(-\frac{M+m}{M-m}\right)\right|^{2n}} \|f_0 - f\|^2, \qquad (1)$$

$$K_i = E_i\left(\int_a^b x^2(t)dt\right); \qquad \frac{1}{\left|T_k\left(-\frac{M+m}{M-m}\right)\right|} = \max_{m \leqslant \lambda \leqslant M} |R_k(\lambda)|.$$



Using LaTeX in this Course…

… will be straight-forward because I will give you templates to work with

BUT you still need to become familiar

with its use by the time you turn in

your 1st homework assignment!

I will now answer your questions! ☺

Review of Some Linear Algebra

We will review some of these together as well

<u>It's a good idea to re-acquaint yourselves with:</u>

- Solving N equations, N unknowns (**Ax = b** setup)
- Matrix view vs. Column view
- The different ways to multiply matrices
- How to find inverse, transpose matrices
- Special matrices: identity (I), upper-triangle (U), lower-triange (L)
- The determinant of a matrix
- The eigenvalues and eigenvectors of a matrix

Matrix Multiplication

*BTW, is this a **Matrix**? Or a **Vector**?*

- Recall:

Matrix Multiplication

Matrix ***A*** x *Matrix* ***B*** = *Matrix* ***C***

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

*Since row1 x column1 is: 1x1 + 1x2 = **3***

*Since row2 x column1 is: 1x1 + 2x2 = **5***

*Since row3 x column1 is: 3x1 + -4x2 = **-5***

3x2 (3 rows, 2 columns) *2x1* *3x1*

- You can only multiply 2 matrices if
  the no. of columns of the *multiplier* = the no. of rows of the *multiplicand*

- That is, if the dimensions are a_x**m** and **m**$_x$b
  - Which results in a matrix of dimensions **a**$_x$**b**

N Linear Equations in *N* Unknowns

Example: How can we solve:

$$\begin{cases} 2x - y = 0 \\ -x + 2y = 3 \end{cases}$$

Using classical algebra?

Using matrix algebra?

Using Column view (vector analysis)

Regular Algebra

$$\begin{cases} 2x - y = 0 & (1) \\ -x+2y = 3 & (2) \end{cases}$$

From (2): $x = 2y - 3$ *(3)*

Use (3) in (1): $2(2y - 3) - y = 0 \Rightarrow 3y - 6 = 0 \Rightarrow \underline{\mathbf{y = 2}}$

Substitute result in either (1) or (2) and get: $\underline{\mathbf{x = 1}}$

Is this a unique solution to this system?

Using Matrix Algebra

- In the form of **Ax = b**

$$\begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 0 \\ 3 \end{bmatrix}$$

equivalent to

$$2x - y = 0$$
$$-x+2y = 3$$

Multiplying *an equation in a system with a scalar gives you a new equation that is also "true" about the system.*

Adding 2 *equations together in a system does the same also!*

- Using **Gaussian Elimination**, we take advantage of certain Algebra rules:

$$\begin{matrix} row_0 \\ row_1 \end{matrix}\left[\begin{array}{cc|c} 2 & -1 & 0 \\ -1 & 2 & 3 \end{array}\right] \rightarrow \left[\begin{array}{cc|c} -1 & 2 & 3 \\ 2 & -1 & 0 \end{array}\right] \rightarrow \left[\begin{array}{cc|c} -1 & 2 & 3 \\ \mathbf{0} & 1 & 2 \end{array}\right] \rightarrow \left[\begin{array}{cc|c} 1 & \mathbf{0} & 1 \\ \mathbf{0} & 1 & 2 \end{array}\right]$$

Augmented Form | *Switched rows* | $row_1 = 1/3 x row_0 + 2/3 x row_1$ | $row_0 = -row_0 + 2 x row_1$

- So, this means that our system can be re-written as: $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$

SO:
x = 1, y = 2

Your TO DOs!

- Make sure you are on Gradescope and Piazza **TODAY!!**

- Do the readings
  - Read the syllabus
  - See Canvas under "Modules" → "**Week 1**" for what to go over…

- Come to class on Wednesday!
- Go to lab/section on Thursday!

- Start on your 1st assignment that's due by SUNDAY

</LECTURE>