Scientific Computing

The Foundations

Alexander G. Ororbia II

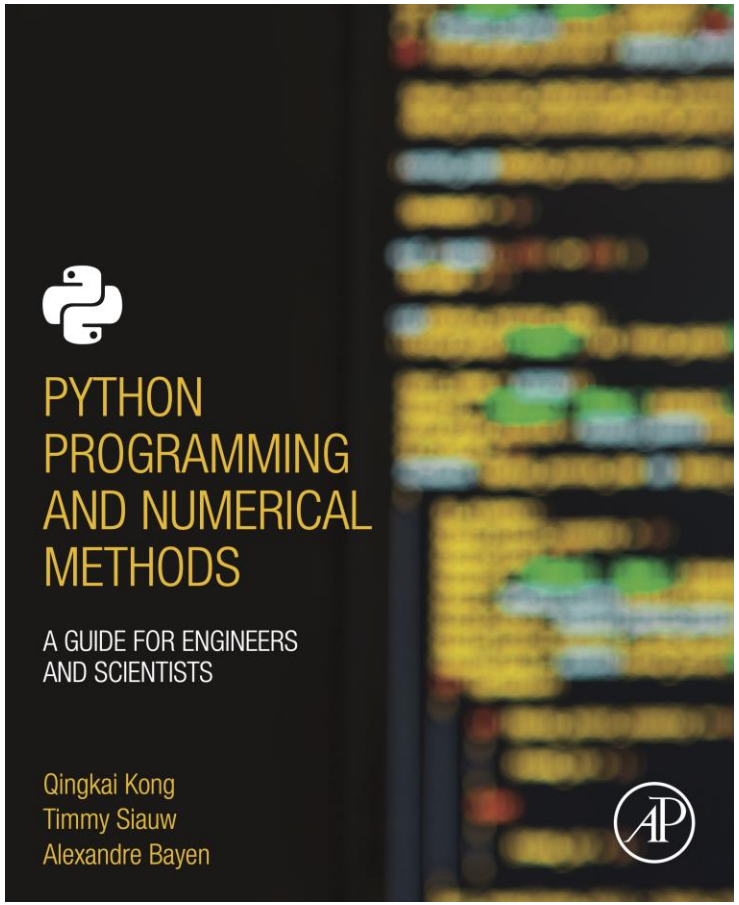
COGS-621: Foundations of Scientific Computing

8/26/2025

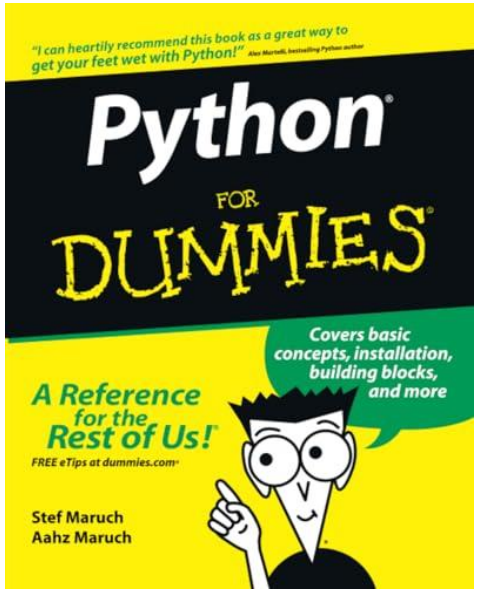
Course Page & Syllabus

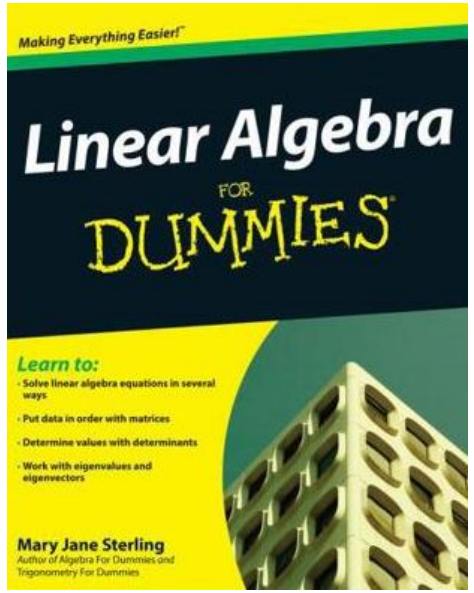
- Syllabus and policy:
  - https://www.cs.rit.edu/~ago/courses/cogs621/index.html
- Prerequisites:
  - COGS-600 and PSYC 640 (or PSYC 717)

Your textbook guide for this class!



Companion Recommendations (good to have on your own shelf)!

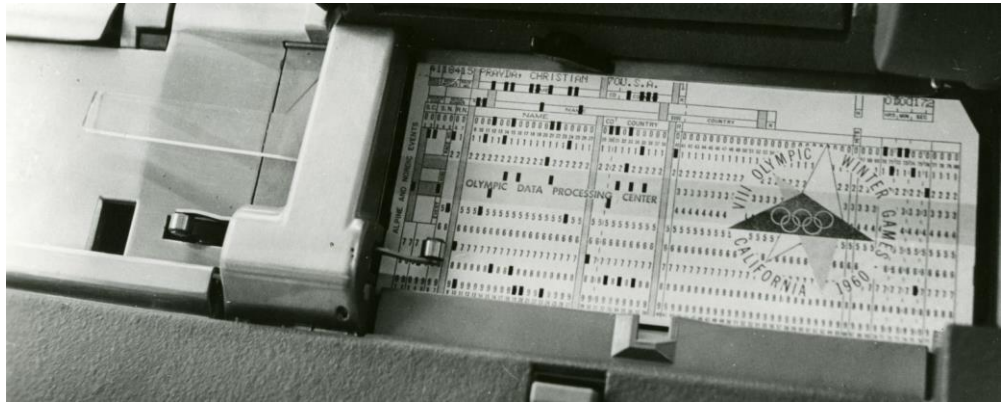




What is computing?

- Manifestation of counting or calculating
  - Goal-oriented activity that requires calculation machinery
  - “Computing” can be done on many mediums (philosophically)
    - Rocks + falling water + toilet paper, a group of coordinated humans, a difference engine, a von Neumann architecture, a neuromorphic crossbar
- Study of and experimentation with algorithmic processes and development of software and hardware

The talented, brilliant women of the (early/pre-NASA) Jet Propulsion Laboratory (JPL) were known as human “computers”.

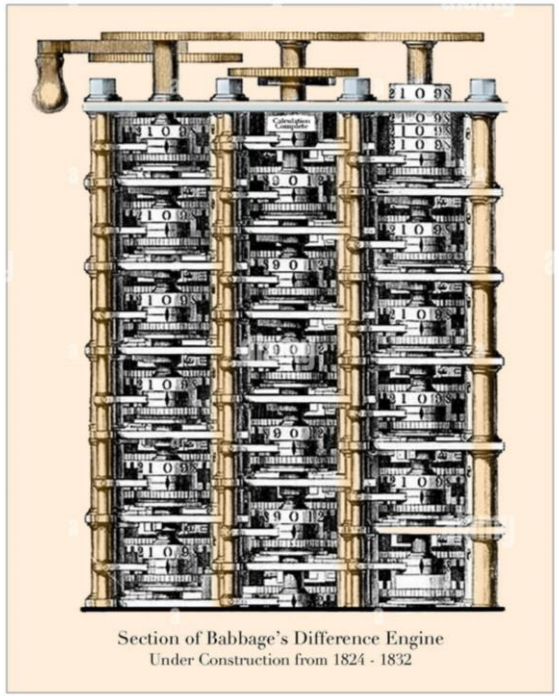


The punch(ed) card, for storing digital information via presence / absence of holes in predefined positions

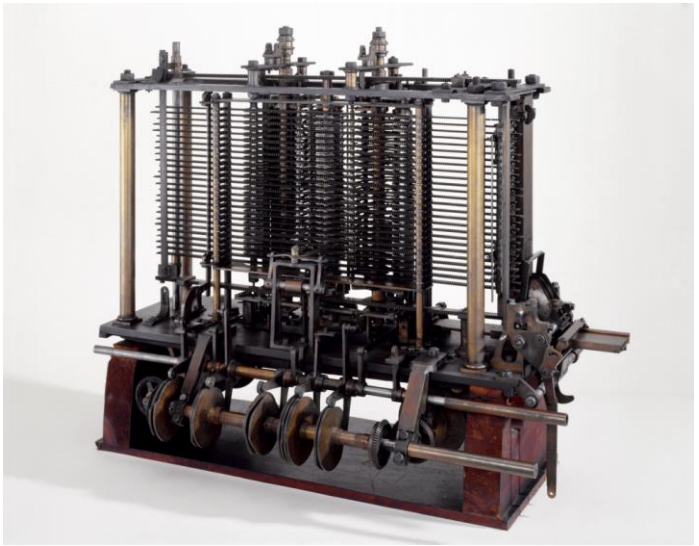
Computation's history

- Difference engine ("calculator")
  - Powered by crank handle
  - Approximated polynomial functions (via tabulating logarithmic / trigonometric functions)

- Analytic(al) engine
  - Incorporated arithmetic logic unit, control flow (conditional branching, loops), integrated memory
  - First general-purpose computer design


Section of Babbage's Difference Engine
Under Construction from 1824 - 1832

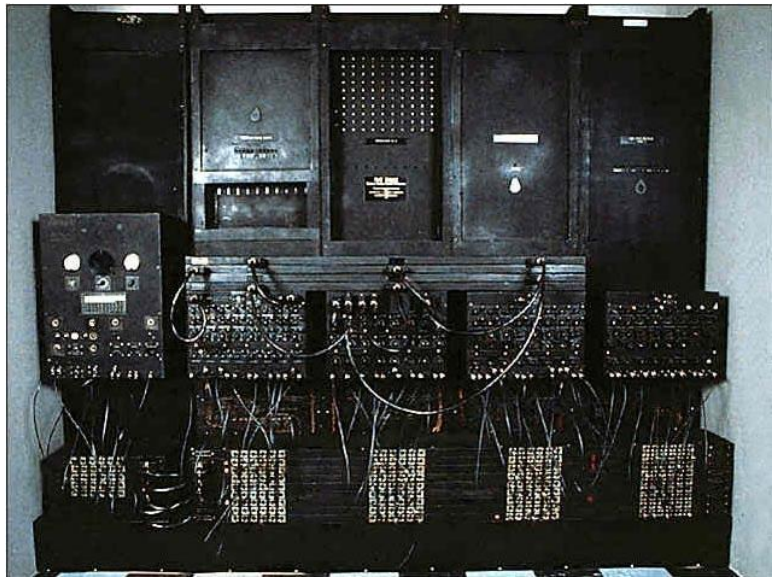

Ada Lovelace


The analytical engine (1849, 2002)

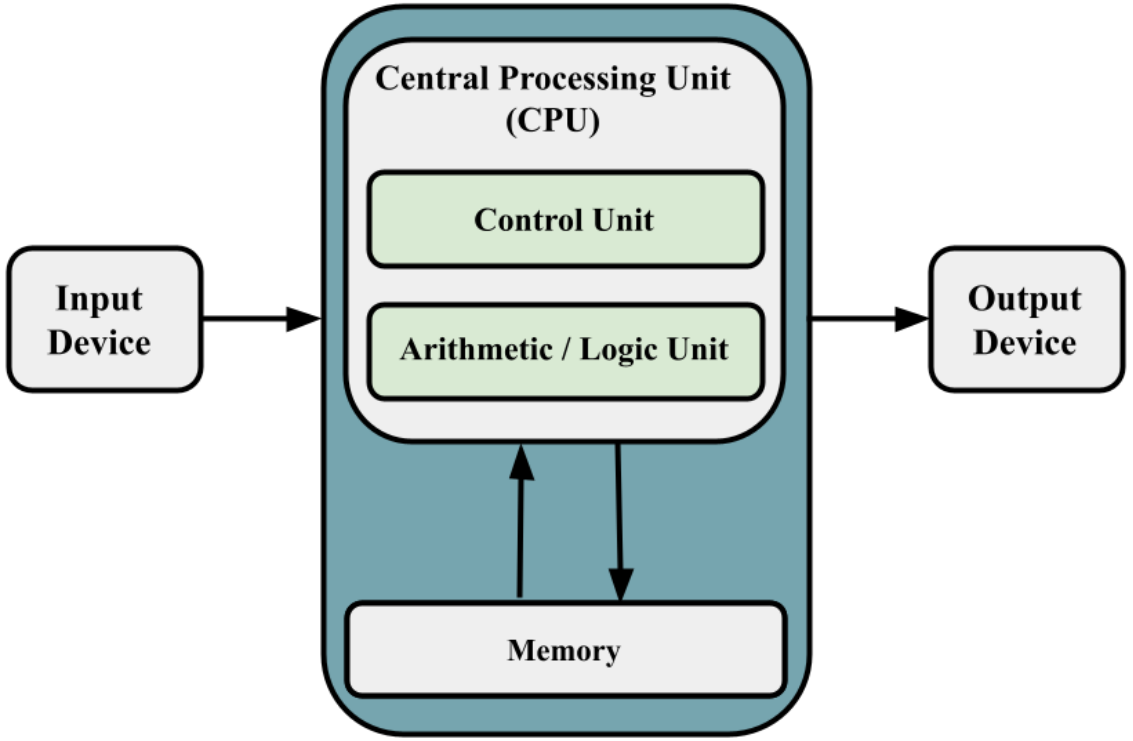

Charles Babbage

Analytic machines and digital computing

- ENIAC (Electronic Numerical Integrator and Computer, 1945)
  - Multiple panels/modules (accumulators, 10-digit decimal memory), branching
- A von Neumann design (EDVAC, 1945)
  - Processing unit (ALU, processor registers), control unit (instruction register, program counter), memory/external mass storage, input/output mechanisms



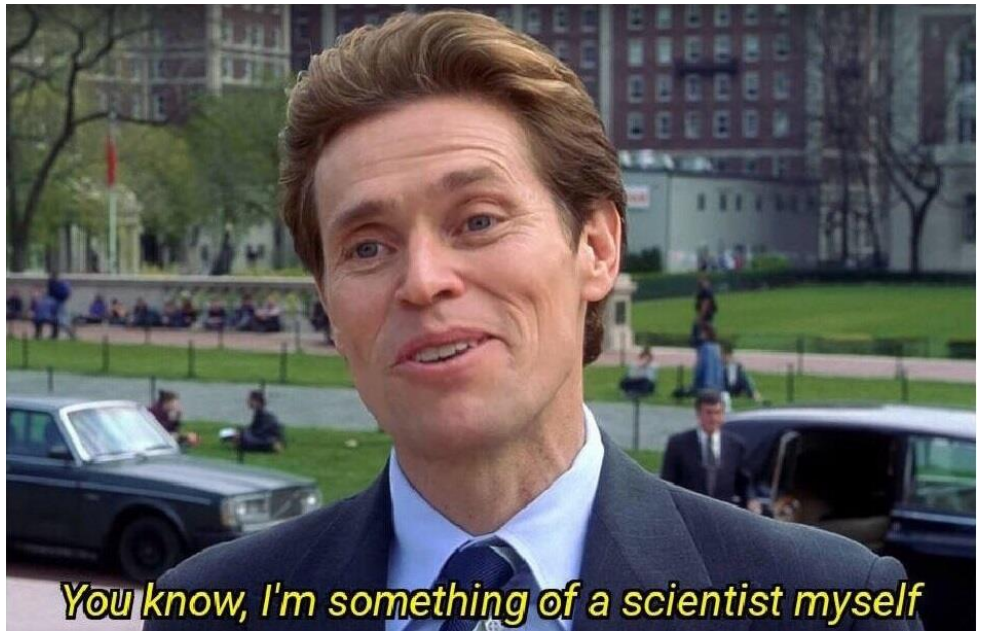
The ENIAC



John von Neumann

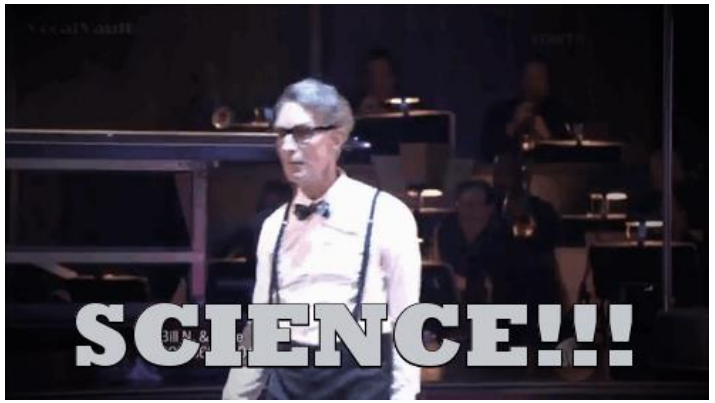
Now, what is science?

- A systematic way to build and organize knowledge
  - About phenomena, the universe
- Construct testable / verifiable hypotheses about the universe around us
  - We make predictions and then test them (refutation or validation)



So, what is scientific computing?

- It is *computing* to support *science* (!)
  - Using machinery of counting/calculation to aid in: refuting/validating hypotheses, modeling a natural stochastic data-generating process



- Scientific method (making use of computation):
  - Ask a question (exploratory data analysis)
  - Formulate a hypothesis (use a model)
  - Design an experiment to test hypothesis (simulation)
  - Analyze data (fit a model, perform uncertainty quantification)

What are we going to learn this semester?

- Lots of good things!
  - Linear algebra
  - Optimization / calculus
  - Differential equations
  - Some forms of statistical analysis/modeling & sampling
  - A tiny bit of Bayesianism
  - A bit of (computational) neuroscience along the way
    - Spiking neural networks (Guest lecture! William)
    - Predictive coding (Guest lecture! Faeze)
    - Active inference graphical models (Guest lecture! Viet)

- Our vehicle = the Python programming/scripting language
  - With some Bash “ducktape” as needed
  - With a little bit of the ngc-learn library (for neuroscience things later)

This class's "slant"

- While the concepts / principles we cover will be generally applicable, we will have somewhat of a bias in this particular offering
  - Our slant = ***computational neuroscience***
  - Largely, this is due to the fact that I am such a scientist
  - Will help us examine some examples where these tools/schemes are applied

- Computational neuroscience
  - One dimension of the larger enterprise of cognitive science/neuroscience
  - Requires many of the tools we will cover in COGS-621
  - For example:
    neuronal dynamics are often expressed through *differential equations*

This class's "slant"

- While the concepts / principles w… pplicable, we will have somewhat of…
  - Our slant = ***comp…***
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  - Will help us ex… e applied

- Computational n…
  - One dimension o… science/neuroscience
  - Requires many of… COGS-621
  - For example: neuronal dynamics… ten expressed through *differential equations*

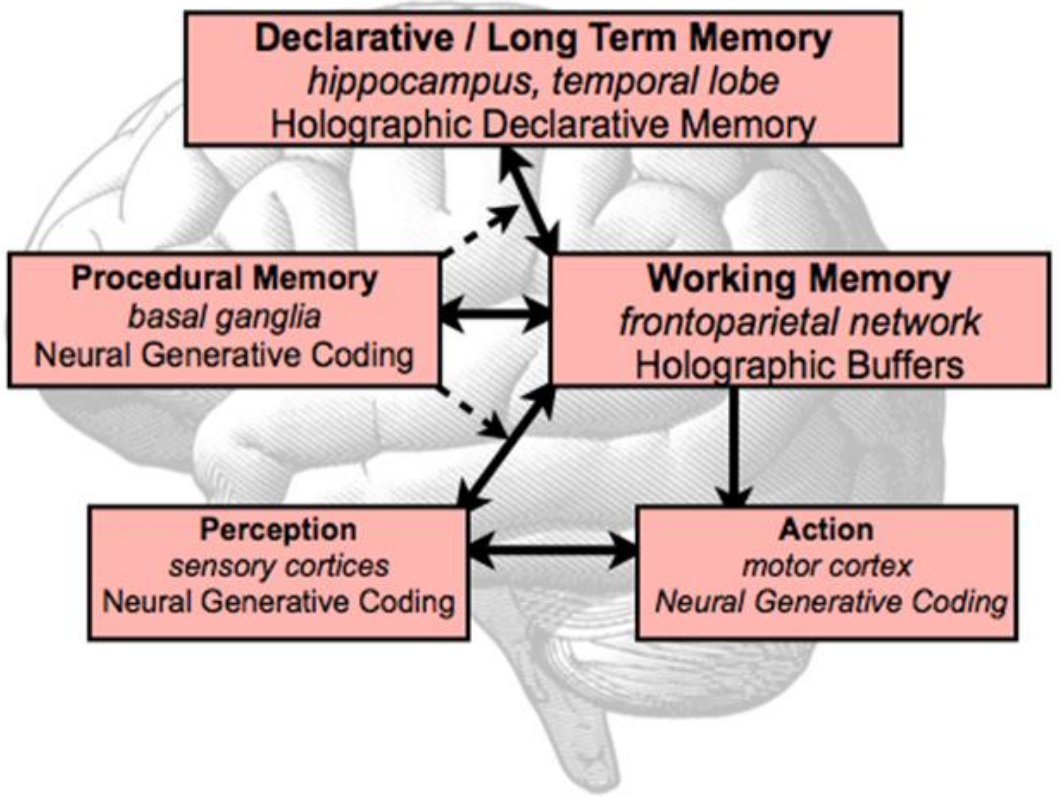
So…now you know the truth…you got stuck with the one loony computational neuroscientist this semester at RIT.

Yay! Lucky you!!

Computational neuroscience at a glance

- Study and investigation of brain function using mathematical, computational tools / theories
  - Interdisciplinary study that draws from:
    - Electrical engineering
    - Computer science
    - Physics
    - Neurobiology
    - Cognitive (neuro)science
  - ***Goal***: to model and understand how nervous systems process information

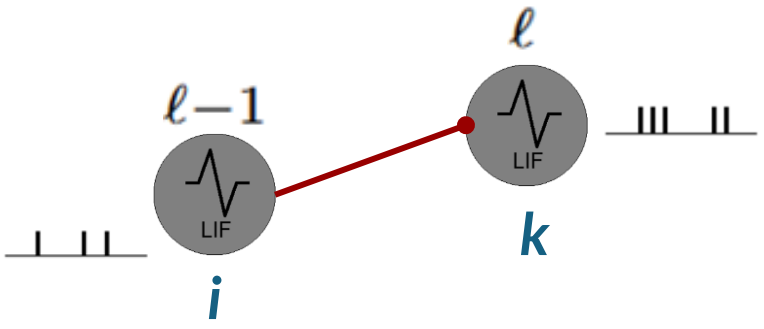
- <u>Focus</u>: descriptions of biologically-plausible/grounded neurons as well as neuronal systems
  - Attention paid to physiology, constraints, and dynamics

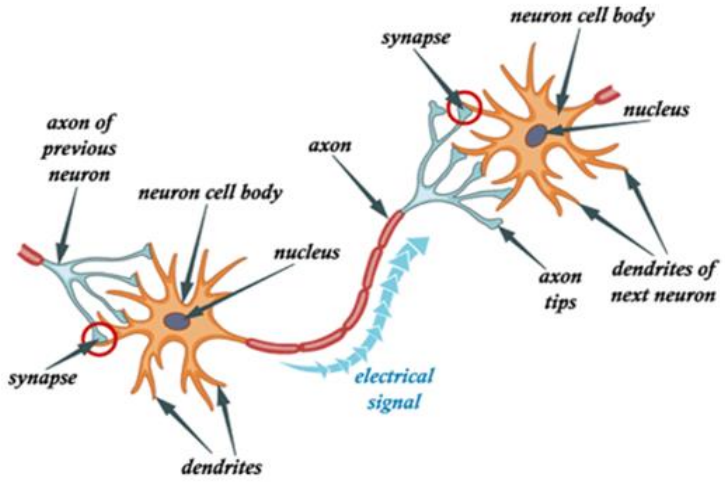


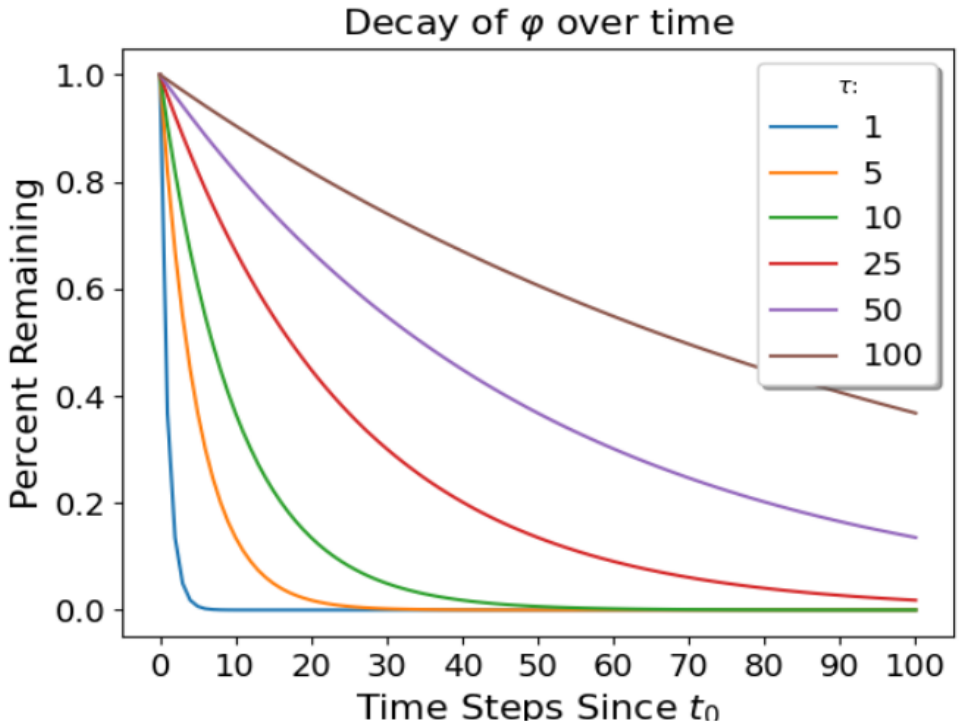
(Ororbia and Kelly, 2021; 2022; 2023)

An example: The leaky integrator

- We can model neuronal cell membrane potential (voltage) via ordinary differential equations (ODEs)
  - Shows change in voltage potential for a given time
  - Popular initial choice: the leaky integrator





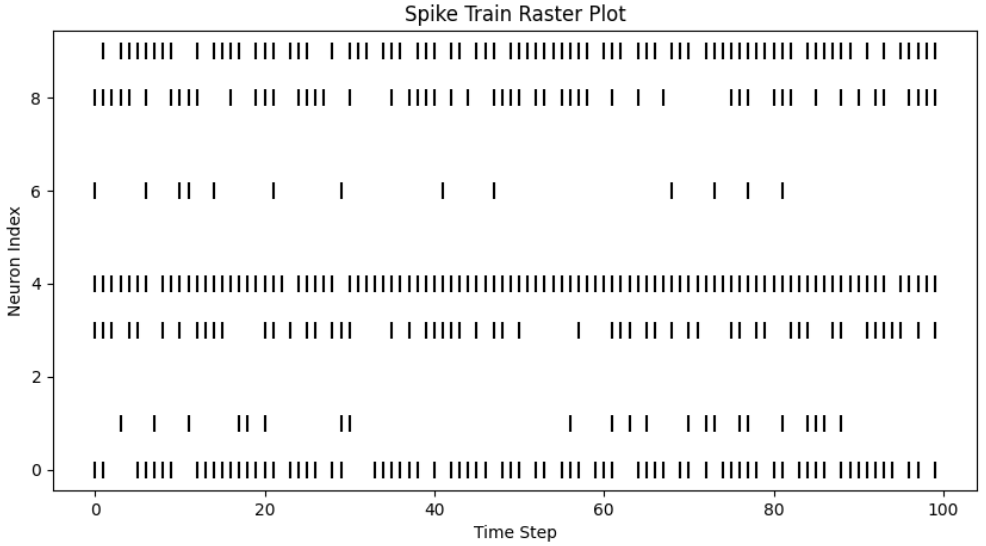


$$\tau_m \frac{\partial v_k^\ell(t)}{\partial t} = -\gamma_v \left(v_k^\ell(t) - v_{rest} \right) + R^\ell j_k^\ell(t)$$

An example: Spiking neural assemblies

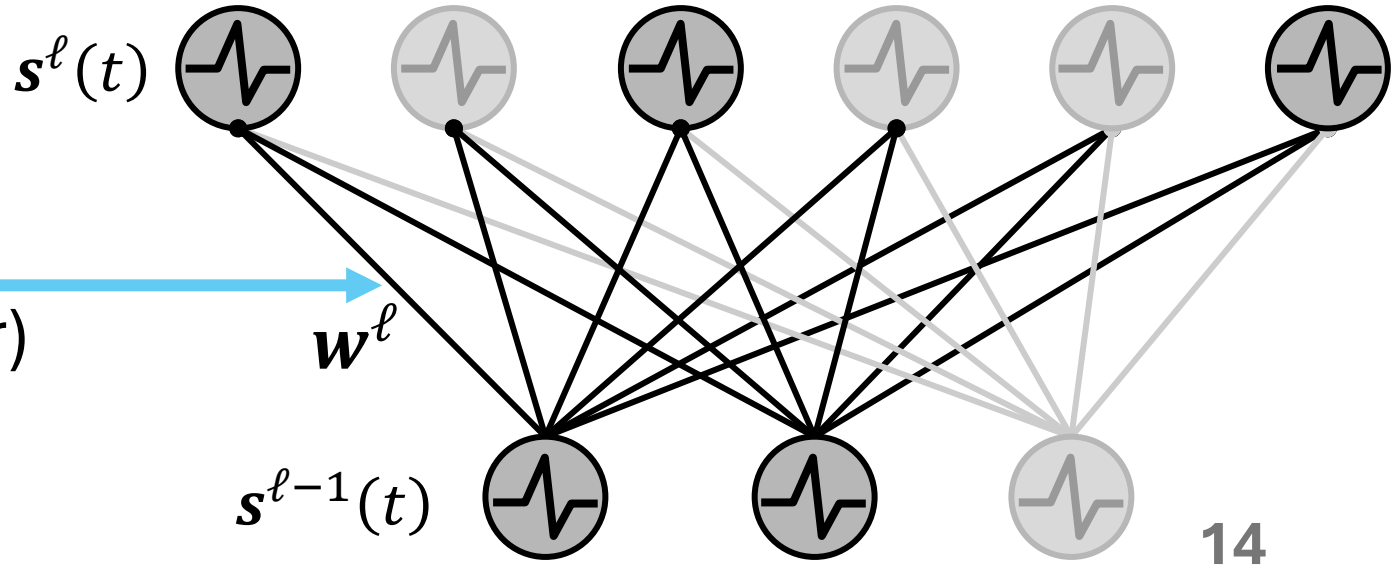
- Synapses (or “efficacies”)
  - We can model electrical current injected into *k*-th neuron in layer ℓ via linear algebra:
    - $j_k^{\ell}(t) = \boldsymbol{w}^{\ell} \cdot \boldsymbol{s}^{\ell-1}(t)$
    - A dot product ($\cdot$) in the above case (bold font denotes vector)

Instantaneous point-wise current



A raster plot

We want to craft assemblies (or connected populations) of these neuronal units!

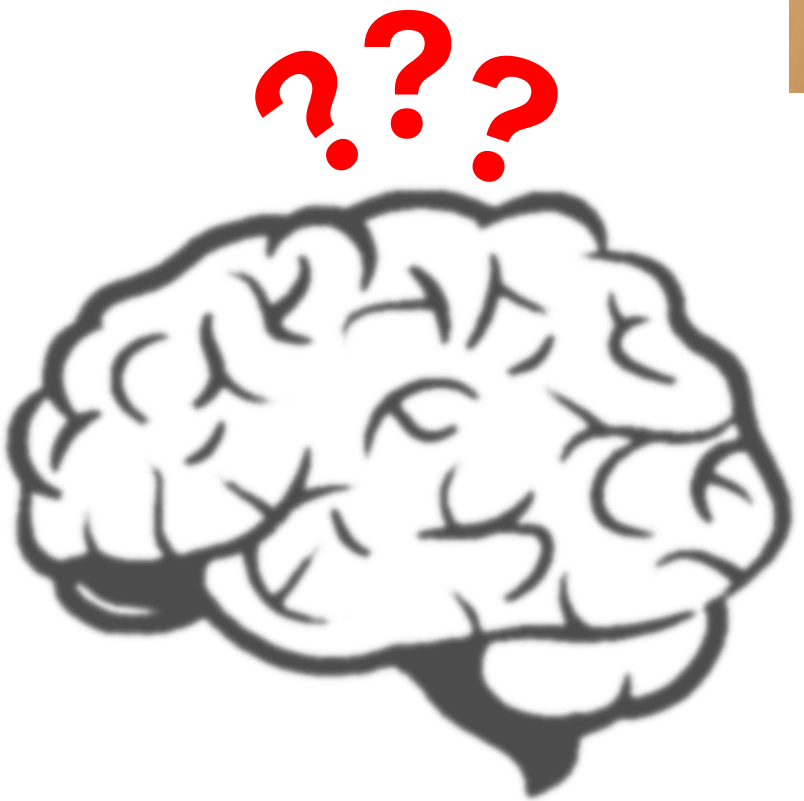


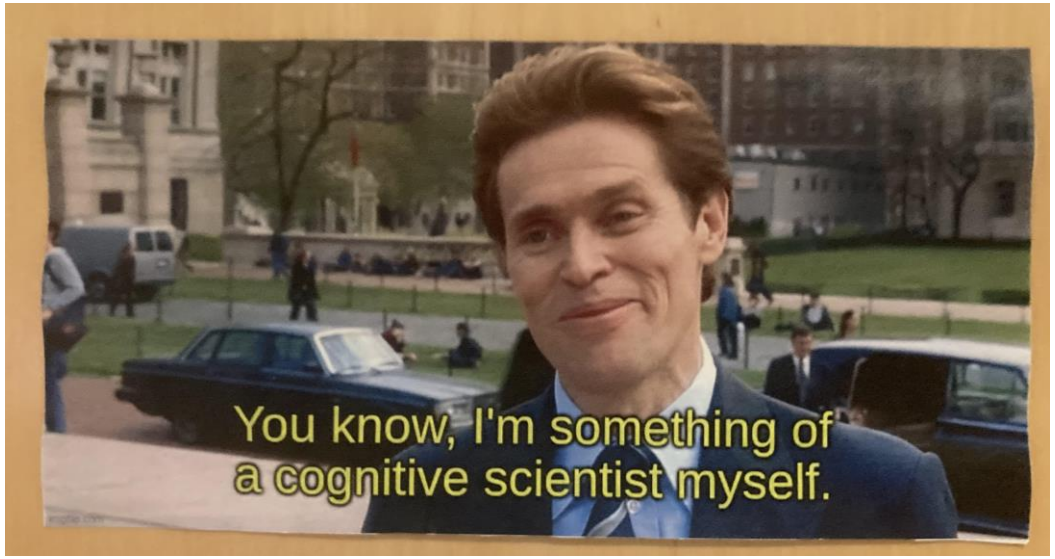
No Class this Thursday, 8/28

- No class this Thursday; I have been called away to participate in a NeuroAI think-tank for NSF

- ***Homework for this/next week***:
  Read Chapter 1-2 of your textbook
  Set up a Python environment (see Chapter 1)
  Create a Github account (free)

Questions?





(Image source: Prof O's office door)

References

- Ororbia, Alexander, and M. Alex Kelly. "A Predictive Processing Implementation of the Common Model of Cognition." *Neuropsychologia* 48.7: 1948-1957.
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- Ororbia, Alexander G., and Mary Alexandria Kelly. "A neuro-mimetic realization of the common model of cognition via hebbian learning and free energy minimization." *Proceedings of the AAAI Symposium Series*. Vol. 2. No. 1. 2023.