Introduction to Scientific Computing

PSCB57
Fall 2018

Professor Hanno Rein

Lecture
Mondays, 9 am - 11 am, MW 160
- The lectures start prompt at ten past the hour.
- Please be on time.

Tutorial
Tuesdays, 3:00 pm - 6:00 pm, SW 505 B
- Space is limited, please come to the tutorial in which you are enrolled in.

E-mail
`hanno.rein@utoronto.ca`
- My e-mails only get delivered three times a week (Mondays, Wednesdays, Fridays, at 9am).
- Please use your university e-mail account when inquiring about the course.

Website
`https://rein.utsc.utoronto.ca/`

Office hours
Mondays 11:30 - 12:00 (SW504C)
Tuesdays 13:00 - 14:00 (SW504C)

Reading/ Bibliography
- Last year's lecture notes, `http://rein.utsc.utoronto.ca/`
- Computational Physics at UofT `http://compwiki.physics.utoronto.ca/`
- Computational Physics, Mark Newman
- Numerical Recipes, The Art of Scientific Computing, 2007, William H. Press
- Learning Python, 5th Edition, Mark Lutz, O'Reilly Media
- Charles Dyer's lecture notes, `http://pathfinder.utsc.utoronto.ca/~pscb57/`
- What every programmer should know about floating point numbers, `https://blogs.oracle.com/darcy/resource/OSCON/OSCON_2015-floating-point.pdf`
- The internet! You can find many resources on the topics that we will cover online.

Software
In this course, we will work with version 3.5 of the programming language `python`. The differences between the `python` versions are small, however, all your submitted work must work with `python` 3.5.

For the assignments, you need to have access to a computer with `python`. If you own a personal computer, please install `python`, `numpy`, `scipy`, `matplotlib`, and `jupyter-notebook`. You are strongly encouraged to get all the software installed before the beginning of the course. You can do this in many different ways. For beginners, the `anaconda` distribution is recommended. For instructions on how to install anaconda see `http://continuum.io` or `http://compwiki.physics.utoronto.ca/`.

Having all the software on your personal computer will make it significantly easier for you to work on the course assignments. However, you can also use computers at UTSC if you do not have a personal computer. The computers in the physics

labs (5th floor of the Science Wing) have `python` installed. You are welcome to use these rooms at any time if there is no other lab is scheduled in the room.

Lectures

I will use the blackboard to derive the mathematical parts of the material. I will only occasionally use slides. The practical part of the lectures will be done using a live demonstration on a computer. Due to the use of different media, you are encouraged to take notes. Reading only the lecture notes will not adequately prepare you for the assignments and exams.

Lecture notes from previous years are available online. However, not that the course content changes a lot from year to year.

Each lecture is two hours long. Please be on time. We start promptly at ten past the hour. We will have a 10 minute break after 50 minutes.

If something is unclear during a lecture or you would like to hear something again, please raise your hand and ask. Ask as many questions as you like. There are no stupid questions and the more questions you ask the better.

As a courtesy towards me and your fellow classmates, please refrain from eating any food during the lecture. Please turn off the sound of all your electronic devices. If your phone rings during the lecture, you will be asked to leave.

Tutorials, assignments, and tests

The tutorials have three purposes:

1. You can ask questions about the course material.
2. You can get help with the current assignment.
3. There will be short tests to asses your understanding of course material and submitted assignments.

Attendance is mandatory whenever a test is scheduled. The format and length of the tests will vary. However, if you do not show up, your mark for both the assignment and the test will be 0.

The deadlines for the submissions of assignments are hard deadlines. Late submissions will not be accepted because the TA will have to grade your submission within a short timeframe. You are required to submit the assignment electronically. How to do this will be discussed in the first lecture.

Most importantly, *if you submit a solution to an assignment, you have to understand it.* After submitting each assignment, you might have to either pass a test or explain your solution to the TA or professor. This is to ensure that you have done the assignment by yourself and did not just copy the solution from a friend or the internet.

Project

You will have the opportunity to work on a project in this course. You can work on the project by yourself or with one other student. Larger teams are not possible.

Each student or team will receive an ESP8266 micro-controller for the project. I will also provide you with any additional sensors or electronic materials you might need. You will also be able to use the physics labs for all your soldering and other hacking needs. In addition to the TA and professor, our Physics Teaching and Research Laboratory Coordinator, Kevin Hurley, will be able to assist you with some technical support.

Grading Scheme

There are three necessary conditions for passing this course:

1. A final grade of at least 50%.
2. A combined grade in all assignments and tests of at least 40%.
3. You have to write the final exam and get at least a 40%.

The final grade will be calculated from all assignments, tests, the midterm, the final exam, and optionally the project. The ratio is as follows:

Assignments and tests	1/4
Midterm	1/4
Final exam	1/2

If you choose to work on the optional project, your grade might increase by up to 2 steps. For example, if you have an A- without the project and manage to accomplish an exceptionally good project, your final grade might be increased up to an A+. Similarly you might be able to increase your grade from a B to an A-. You cannot use the project to increase a failing grade (F, lower than 50%) to a passing grade. You need to decide if you want to work on a project by **October 16th**.

If you miss the midterm or a test for a valid reason (see below), your final exam will be worth more. However, if you miss the midterm or a test for a non-valid reason, it will be counted as zero points. It is not possible to retake a test or midterm at a later date.

The final exam may include, but is not restricted to, material from all lectures, assignments, and tutorials. Neither a calculator nor an equation sheet will be allowed. Don't worry, you won't need them. The exam will focus on your understanding of the subject, rather then long mathematical calculations.

Learning outcomes

The learning outcomes in this course are broad and diverse. It is not enough to memorize course material and then pass a final exam. This is really important, so let me repeat it: **To succeed in this course you need to engage in the lectures, assignments and projects.**

Specifically, I expect that you

1. are comfortable writing small python programs.
2. can use jupyter notebooks.
3. can visualize data using matplotlib.
4. understand the concepts and limitations related to floating point numbers.
5. know how to use numpy and work with arrays.
6. understand chaotic maps, how to calculate them, and how to interpret their behaviour.
7. know several root finding algorithms and their differences.
8. know the basic building blocks of a computer.
9. can numerically approximate an integral or a derivate.
10. know methods to integrate a set of ordinary differential equations.
11. understand the concepts of random number generators, random sampling and Monte Carlo methods.

Absences

In the case of a problem that supports an absence to a tutorial session or an inability to hand in an assignment before the deadline, your grade will be calculated on the basis of all other tutorial work. In the case of a problem that supports the absence to the midterm, your grade will be calculated by increasing the weight of the final exam. Valid and *official supporting documentation* must be submitted within five business days of the missed tutorial or test. It is your responsibility to hand in documentation on time. Failure to do so will impact your grade.

Accessibility

Students with diverse learning styles and needs are welcome in this course. In particular, if you have a disability/health consideration that may require accommodations, please feel free to approach me and/or the AccessAbility Services Office as soon as possible. I will work with you and AccessAbility Services to ensure you can achieve your learning goals in this course. Enquiries are confidential. The UTSC AccessAbility Services staff (located in SW302) are available by appointment to assess specific needs, provide referrals and arrange appropriate accommodations (416) 287-7560 or `ability@utsc.utoronto.ca`.

Academic Integrity

Academic integrity is one of the cornerstones of the University of Toronto. It is critically important both to maintain our community which honours the values of honesty, trust, respect, fairness and responsibility and to protect you, the students within this community, and the value of the degree towards which you are all working so diligently. Detailed information about how to act with academic integrity, the Code of Behaviour on Academic Matters, and the processes by which allegations of academic misconduct are resolved can be found online: `http://www.artsci.utoronto.ca/osai/students`.

According to Section B of the University of Toronto's Code of Behaviour on Academic Matters (`http://www.governingcouncil.utoronto.ca/policies/behaveac.htm`) which all students are expected to know and respect, it is an offence for students to:

- To use someone else's ideas or words in their own work without acknowledging that those ideas/words are not their own with a citation and quotation marks, i.e. to commit plagiarism.
- To include false, misleading or concocted citations in their work.
- To obtain unauthorized assistance on any assignment.
- To provide unauthorized assistance to another student. This includes showing another student completed work.
- To submit their own work for credit in more than one course without the permission of the instructor.
- To falsify or alter any documentation required by the University. This includes, but is not limited to, doctor's notes.
- To use or possess an unauthorized aid in any test or exam.

Specifically to this course, please be reminded that you need to understand every assignment that you submit. If you work together on an assignment and you do not pass the post-assignment test, this is a warning flag and suggests that you might have not done the assignment yourself.

There are other offences covered under the Code, but these are by far the most common. Please respect these rules and the values which they protect. Offences against academic integrity will be dealt with according to the procedures outlined in the Code of Behaviour on Academic Matters.

Tentative Class Schedule

	Date	Topic
Tutorial 1	Sept. 4th	**Python/jupyter notebook installation.** In the first tutorial, we will help you setup python and jupyter notebooks on your own personal laptop or how to use these tools on one of the physics lab computers. If you have not used python before, it is essential that you come to this tutorial as you will not be able to work on the assignments otherwise.
Lecture 1	Sept. 10th	**Introduction to Python.** In the first lecture, you will learn the basics about python, the python syntax, and the features of jupyter notebooks. After this lecture you should be able to write and run simple python programs.
Tutorial 2	Sept. 11th	**Test 1.** In the second tutorial, you will need to demonstrate to the TA that you are able to write and run a short python program. You can either do this on your own personal computer or on one of the computers in the physics labs. The TA might give you a simple task such as *"Write a python program that prints out the result of* 5×98*"*. Once you have completed the task successfully, you may leave the tutorial. The purpose of this test is to ensure everyone is able to work on the assignments which follow. The test is worth **10pts**.
Lecture 2	Sept. 17th	**Number representations.** In this lecture, we will discuss how numbers are represented on a computer. In particular, we will discuss IEEE754 floating point numbers in great detail. You will be able to determine how accurate a calculation might possible be on a computer and when a calculation might fail completely. You should understand how one can convert from decimal numbers to floating point numbers and back. Assignment 1 will be about floating point numbers.
Tutorial 3	Sept. 18th	**Drop in help desk.** In this tutorial you will have the opportunity yo ask questions and get help with assignment 1. Attendance is voluntary for this tutorial.
Assignment 1	Sept. 24th	**Deadline to hand in assignment 1 is 9am!** Assignment 1 is worth **10pts**.
Lecture 3	Sept. 24th	**Arrays, plotting, and chaotic maps.** Using the logistic and standard map, we will explore two chaotic iterative maps. While working with these systems, you will learn how to make plots in python with matplotlib and how to use scientific python libraries such as numpy. You will use these tools to complete assignment 2.
Tutorial 4	Sept. 25th	**Test 2.** In this tutorial you will go over your submission of assignment 1. Make sure you really understand your submission. Although having a working program is good, it is not sufficient to get marks in the test. You might have to explain parts of your program to the TA or professor. In addition to the assignment, the test is worth **10pts**.
Assignment 2	Oct. 1st	**Deadline to hand in assignment 2 is 9am!** Assignment 2 is worth **10pts**.
Lecture 4	Oct. 1st	**Root finding methods.** You will learn how to solve one dimensional non-linear equations using a root solver. We will discuss different root solvers and their properties. You will also learn how to numerically solve non-linear problems in higher dimensions and what problems might arise.
Tutorial 5	Oct. 2nd	**Test 3.** In this tutorial you will go over your submission of assignment 2. Make sure you really understand your submission. Although having a working program is good, it is not sufficient to get marks in the test. You might have to explain parts of your program to the TA or professor. In addition to the assignment, the test is worth **10pts**.

October 8th to Oct. 12th – Reading week – No lectures or tutorials		
Lecture 5	Oct. 15th	**Computers and micro-controllers.** In this lecture we'll take a step back and discuss what a computer actually is. You will learn the basic components that make up a computer. As an example of a very small computer, we will discuss the ESP8266 micro-controller. You will be able to use this micro-controller for an optional project in this course.
Tutorial 6	Oct. 16th	**Project.** Attendance for this tutorial is optional. Come if you are interested in doing an optional project using the ESP8266 micro-controller. If you do a succseful project, your grade might get a boost (see above). After you present your idea for the project to the TA or professor, **you can sign up for the project** and can pick up a WEMOS D1 mini device with an ESP8266 micro-controller and any additional components you might need.
Assignment 3	Oct. 22nd	**Deadline to hand in assignment 3 is 9am!** Assignment 3 is worth **10pts**.
Lecture 6	Oct. 22nd	**Numerical integration and differentiation.** You will learn how to solve integrals numerically on a computer. We will discuss the rate of convergence of different algorithms. We will also cover how to calculate finite differences.
Tutorial 7	Oct. 23rd	**Test 4.** In this tutorial you will go over your submission of assignment 3. Make sure you really understand your submission. Although having a working program is good, it is not sufficient to get marks in the test. You might have to explain parts of your program to the TA or professor. In addition to the assignment, the test is worth **10pts**.
Midterm	Oct. 29th	**Midterm** In the first hour of the Monday morning lexture, you will write the midterm exam. After the midterm, we will have a short break and then continue with the lecture.
Lecture 7	Oct. 29th	**Differential equations and dynamical systems.** You might have taken a course on differential equations before. If so great. If not, then this lecture will provide you a basic idea of what differential equations are and where they occur. We will discuss how differential equations arise in dynamical systems and how typical solutions look like.
Tutorial 8	Oct. 30th	**No tutorial.** There is currently no tutorial scheduled during this week. There will be an announcement in class should there be a need for a tutorial related to differential equations.
Assignment 4	Nov. 5th	**Deadline to hand in assignment 4 is 9am!** Assignment 4 is worth **10pts**.
Lecture 8	Nov. 5th	**Numerical solutions to differential equations.** In this lecture we will continue the discussion of differential equations, but with a focus on solving them numerically. You will get to know the Euler method, as well as higher order Runge-Kutta methods. We will discuss the convergence of these schemes and introduce the 'big O' notation.
Tutorial 9	Nov. 6th	**Test 5.** In this tutorial you will go over your submission of assignment 4. Make sure you really understand your submission. Although having a working program is good, it is not sufficient to get marks in the test. You might have to explain parts of your program to the TA or professor. In addition to the assignment, the test is worth **10pts**.
Lecture 9	Nov. 12th	**N-body simulations.** We discuss N-body simulations, i.e., simulations that predict the motion of planets and stars which are under the influence of mutual gravity. We will use python to run and analyze such simulations. We will find that the simulations are often chaotic, making precise long term predictions impossible.

Tutorial 10	Nov. 13th	**Project.** Attendance for this tutorial required only for those students who have signed up for a project. In the tutorial you will talk to the TA or professor about your progress, show a demo, or get help if you are stuck.
Assignment 5	Nov. 12th	**Deadline to hand in assignment 5 is 9am!** Assignment 5 is worth **10pts**.
Lecture 10	Nov. 19th	**Random numbers and Monte Carlo methods.** In this lecture, we will discuss what random numbers are and how computers generate them. We will then use random numbers to perform numerical calculations. We will discuss how such methods can be used in statistics when solving integrals that appear in Bayes' Theorem.
Tutorial 11	Nov. 20th	**Test 6.** In this tutorial you will go over your submission of assignment 5. Make sure you really understand your submission. Although having a working program is good, it is not sufficient to get marks in the test. You might have to explain parts of your program to the TA or professor. In addition to the assignment, the test is worth **10pts**.
Lecture 11	Nov. 26th	**Projects.** In this lecture you will present the micro-controller projects that you've been working on.
Tutorial 12	Nov. 27th	**Exam prep.** In this tutorial, you will solve several problems from previous exams in small groups, then discuss your answers with the TA or professor. This is for practice only, you will not receive a grade for your answers.
Lecture 12	Dec. 3rd	**Make up lecture / revision.** We will use the last lecture to wrap-up any loose ends. If time permits, we will revisit some of the more difficult material from the course. We will also talk about how to best prepare for the final exam.

End Congratulations! You've read the syllabus all the way to the end. As a reward you will get one extra point counting towards your assignment grade. Just draw a picture of a cat somewhere on the final exam (any stick figure cat with four legs and a tail will do).