Introduction to Scientific Computing

PSCB57
Fall 2017

Professor Hanno Rein

Lecture Mondays, 9 am - 11 am, HW 214
- The lectures start prompt at ten past the hour.
- Please be on time.

Tutorial Tuesdays, 3:00 pm - 6:00 pm, SW 505 B

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Office hours Mondays 11:00 - 12:00
Tuesdays 13:00 - 14:00
or by appointment

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, as well as the Geotab project, 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 your life significantly easier. 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 unless a lab is scheduled.

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.

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 quizzes

The tutorial have three purposes:

1. You can ask questions about the course material.
2. You can get help with the current assignment.
3. You will take quizzes about your assignment. The mark from these quizzes will contribute to your final mark.

Tutorial attendance is mandatory whenever a quiz is scheduled. If you do not show up, your mark for the assignment and quiz will be 0%. There might also be quizzes during the lecture.

The difficulty of each assignment and the contribution towards the final grade will vary. The deadline for submissions will typically be on a Friday. This is a hard deadline. You are required to submit the assignment electronically.

The fraction of submitted and correctly solved problems will constitute towards your grade. 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 quiz or explain your solution to a TA. A low performance in the quiz will nullify your points from that assignment. By the end of the course, your grade in the assignments has to be 40% or higher, otherwise you will not pass the course.

Geotab project

You will work on a team based project where you apply some of the knowledge you learned. Each team will receive a device that plugs into a car and collects data in real time. Your task will be to collect, access, analyze and interpret this real world data set. There will be multiple deliverables related to this project including a project proposal, a final presentation and a report. The grades for these deliverables will contribute 20% of your total mark for this course.

I would like to thank Geotab for kindly providing these devices for this course. Thanks to their help, we can work with a real-world product and real-world data!

Grading Scheme

There are four necessary conditions for passing this course:

1. A final grade of at least 50%.
2. A combined grade in all assignments of at least 40%.
3. You have to write the final exam.
4. You have to work on the Geotab project and hand in a report.

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

Assignments and quizzes	25
Geotab project	20
Midterm	20
Final exam	35
Total	100

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

The final exam will take place during the exam period. The exam may include, but is not restricted to, material from all lectures and all 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 basic interpolation and extrapolation algorithms.
6. know several root finding algorithms and their differences.
7. can numerically approximate an integral.
8. know methods to integrate a set of ordinary differential equations.
9. understand the concepts of random number generators, random sampling and Monte Carlo methods.
10. are able to work with real world data in a team based setting.
11. can pose questions that can be answers with an available data-set.
12. assess the validity of your conclusion taking into account limitations such as measurement errors and the size of the available data-set.

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.

Specificlly to this course, please be reminded that you need to understand every assignment that you submit. If you work together on an assignment, you still have to be able to pass the quizzes in the tutorials.

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

Week	Date	
1	Sept. 11th	Introduction, Python, Assignments, Geotab project
2	Sept. 18th	Floating point representation of numbers
3	Sept. 25th	LU Decomposition
4	Oct. 2nd	Interpolation and extrapolation
—	Oct. 9th	Reading week – no lecture
5	Oct. 16th	Numerical integration
6	Oct. 23th	Differential Equations I
7	Oct. 30th	Differential Equations II
8	Nov. 6th	N-body integrations, geometric integration methods
9	Nov. 13th	Grid-based methods
10	Nov. 20th	Monte Carlo methods
11	Nov. 27rd	tbd
12	Dec. 4th	Geotab project - presentations