E7441: Scientific computing in biology and biomedicine

Overview

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RECETOX

Bibliography:

- KONG Q., SIAUW T., BAYEN A. (2020). Python programming and numerical methods. Academic Press. ISBN: 9780128195499
- HEATH M.T. (2002). Scientific Computing. An introductory survey. McGraw-Hill, 2nd edition. ISBN: 0-07-239910-4 Good accompanying materials at https://heath.cs.illinois.edu/scicomp/notes/index.html, including slides and demos! Used as basis for the first part of the course.
- KEPNER J. (2009). Parallel Matlab for Multicore and Multinode Computers. SIAM Publishing. ISBN: 978-0-898716-73-3
- GENTLE J.E. (2005). Elements of Computational Statistics. Springer. ISBN:978-0387954899

Computing environments for the course:

- PYTHON 3, https://www.python.org - with NUMPY and SCIPY packages
- recommended: JUPYTERLAB for exercises
- suggestion: install PYTHON and related packages using a distribution like ANACONDA or MAMBA for easier integration of dependencies
- R, http://www.r-project.org - "environment for statistical computing and graphics"

WARNING: Some pieces of code shown during the course may not represent the optimal implementation in the given language. They are merely a device for demonstrating some principles.

Overview of the topics:

1. Introduction to scientific computing
2. Systems of linear equations: square and non-square
3. Basic methods for non-linear equations and optmization
4. Stochastic methods (touching upon optimization as well)
5. Basic concepts of parallel computing (in Python)
6. Examples of implementations of various fundamental methods in statistics and machine learning

Organization:

- combined theoretical presentation and practical work
- 4 homeworks and 1 project (i.e. a more consistent homework)
- Project presentations: May 12th, 2025
- Deadline for sending in the homeworks (via email): May 12th, 2025
- Delivery of homeworks and project presentations are required for qualifying for the exam. No homeworks and/or project = no exam
- Final mark: 50% homework and project + 50% exam

Questions?