

BT 2020 — Numerical Methods for Biology

Jan–May 2019

Course Plan

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Lectures

Lectures (Karthik): **B Slot**, Mon (09:00), Wed (13:00), Fri (11:00)
Lectures (Athi): **B Slot**, Mon (09:00), Tue (08:00), Wed (13:00)
Labs/Tutorial: **S Slot**, Thu (14:00 – 16:00) (bring laptops!)
Venue: BT 108
Teaching Assistants: Malvika S (bt15d306@smail / BT-II 201A)
Karthik D (bs14b020@smail / BT-II 211)
Vishnu Narayan (be14b033@smail / BT-II 201A)
Debomita Chakraborty (bt18d301@smail / BT-II 512)
Office hours: By appointment
Piazza: <http://piazza.com/iitm.ac.in/spring2019/bt2020>

Objectives

The main objective of the course is to introduce you to various aspects of mathematical modelling, in the particular context of biological systems. At the end of the course, it is expected that you will have a knowledge of important concepts related to the mathematical modelling of complex systems, especially metabolic networks, protein interaction networks and gene regulatory networks, and will be able to apply them to model the behaviour of biological systems as well as develop strategies for manipulating them.

- Introduce you to fundamentals of scientific computing
- Introduce you to a high-level programming language (MATLAB)
- Learn about various important numerical methods, across a breadth of topics
- Many of which are also specially important in biology
- Improve your programming skills (learn good programming practices)

Coursework and grading

- Attendance to the lectures is required; late-comers will be marked absent
- Consistent performance will be key to a good grade

- Weightage (minor changes may happen):

| | |
|--------------------|-----|
| Quizzes I/II/Pop: | 30% |
| Homework: | 30% |
| End-semester exam: | 40% |

For every hour spent in class, I expect you to spend at the least 2–3 hours outside of class on reading relevant and additional material/programming to understand the concepts. I also expect you to inculcate professionalism and maintain the highest level of integrity.

Important Dates

| Date | Day | Time | Event |
|-----------|-----|-------|--------------------|
| 19-Feb-18 | Tue | 08:00 | Quiz I |
| 4-Mar-18 | Tue | 13:00 | Mid-term feedback |
| 27-Mar-18 | Tue | 08:00 | Quiz II |
| 18-Apr-18 | Thu | 14:00 | Final feedback/TCF |
| 30-Apr-18 | Tue | 09:00 | End-semester Exam |

Homework

There will be many assignments during the course. They will all involve programming in MATLAB. I will give an adequate introduction to MATLAB during the course if requested. Please have a look at this page (from Cosma Shalizi’s blog), on minimal advice to under-graduates on programming: <http://cscs.umich.edu/~crshalizi/weblog/593.html>. All deadlines (homework/project) are usually at 5:00 pm on the date mentioned, unless instructed otherwise, via a Dropbox upload at <http://tinyurl.com/bt2020-submit>.

Late submission penalties: 1 second – 24 h: 20%; 24–48 h: 40%; > 48h: 60%

Early submission bonuses: > 24h: 5%, > 48h: 10%, > 72h: 20%

Evaluation: Assignments will be evaluated by the TAs within two weeks of the due date. You can check out your marks and contest them, if needed, for at most one more week post-evaluation, i.e. three weeks from the due date of the assignment.

Academic integrity

While you can take help from your colleagues on homework, *copying* is not permitted. Copying from anywhere, including the Web is not allowed. Offenders will be penalised letter grades. For example, you can ask your friends for hints if you are stuck, but at no point should you take a look at their code itself. I would much rather that you come to me if you are stuck.

Transgressions are easy to find, and will be reported to the “Sub-committee for the Discipline and Welfare of Students” and will be dealt with very strictly. Mention any collaboration (discussions only!) in your solutions. Note that I take copying extremely seriously, and will not show any mercy.

The Institute guidelines (which I consider lenient) may be found here: http://academic.iitm.ac.in/sites/default/files/Graded_punishments.pdf. You must not carry your mobile phone/e-book reader to the exam desk, even if they have been switched off.

Tentative schedule

| Week | Date | Day | Lecture # | Lab # | Topic |
|------|-----------|-----|-----------|-------|-------------------------------------------------------------|
| 1 | 16-Jan-19 | Wed | 1 | | Administrivia/Introduction to Numerical Methods |
| 1 | 17-Jan-19 | Thu | 2 | | Overview of Approximations and Errors |
| 1 | 18-Jan-19 | Fri | | 1 | Introduction to MATLAB |
| 2 | 21-Jan-19 | Mon | 3 | | Floating-Point Representation |
| 2 | 22-Jan-19 | Tue | | | |
| 2 | 23-Jan-19 | Wed | 4 | | Floating-Point Representation / Introduction to MATLAB |
| 2 | 24-Jan-19 | Thu | | 2 | Introduction to MATLAB |
| 2 | 25-Jan-19 | Fri | 5 | | Matrix Computations for Solving Systems of Linear Equations |
| 3 | 28-Jan-19 | Mon | 6 | | Matrix Computations for Solving Systems of Linear Equations |
| 3 | 29-Jan-19 | Tue | | | |
| 3 | 30-Jan-19 | Wed | 7 | | Matrix Computations for Solving Systems of Linear Equations |
| 3 | 31-Jan-19 | Thu | | 3 | MATLAB / Numerical Methods Basics |
| 3 | 1-Feb-19 | Fri | 8 | | Matrix Computations for Solving Systems of Linear Equations |
| 4 | 4-Feb-19 | Mon | | 4 | MATLAB / Numerical Methods Basics |
| 4 | 5-Feb-19 | Tue | | | |
| 4 | 6-Feb-19 | Wed | | 5 | Matrix Factorisation |
| 4 | 7-Feb-19 | Thu | 9 | | Linear Least Squares |
| 4 | 8-Feb-19 | Fri | 10 | | Linear Least Squares |
| 5 | 11-Feb-19 | Mon | 11 | | Linear Least Squares; Mid-term course feedback due |
| 5 | 12-Feb-19 | Tue | | | |
| 5 | 13-Feb-19 | Wed | 12 | | Eigenvalue Problems |
| 5 | 14-Feb-19 | Thu | | 6 | Linear Least Squares |
| 5 | 15-Feb-19 | Fri | 13 | | Eigenvalue Problems |
| 6 | 18-Feb-19 | Mon | 14 | | Eigenvalue Problems |
| 6 | 19-Feb-19 | Tue | | | Quiz I |
| 6 | 20-Feb-19 | Wed | 15 | | Optimisation |
| 6 | 21-Feb-19 | Thu | | 7 | Eigenvalue Problems |
| 6 | 22-Feb-19 | Fri | 16 | | Optimisation |
| 7 | 25-Feb-19 | Mon | 17 | | Optimisation |
| 7 | 26-Feb-19 | Tue | | | |
| 7 | 27-Feb-19 | Wed | 18 | | Optimisation |
| 7 | 28-Feb-19 | Thu | | 8 | Optimisation |
| 7 | 1-Mar-19 | Fri | 19 | | Optimisation |
| 8 | 4-Mar-19 | Mon | 20 | | Random Numbers and Simulations |
| 8 | 5-Mar-19 | Tue | | | |
| 8 | 6-Mar-19 | Wed | 21 | | Random Numbers and Simulations |
| 8 | 7-Mar-19 | Thu | | 9 | Optimisation |
| 8 | 8-Mar-19 | Fri | | | |
| 9 | 11-Mar-19 | Mon | 22 | | Solution to non-linear equations |
| 9 | 12-Mar-19 | Tue | 23 | | Solution to non-linear equations |
| 9 | 13-Mar-19 | Wed | 24 | | Solution to non-linear equations |
| 9 | 14-Mar-19 | Thu | | 10 | Random Numbers |

| Week | Date | Day | Lecture # | Lab # | Topic |
|------|-----------|-----|-----------|-------|-------------------------------------------|
| 9 | 15-Mar-19 | Fri | | | |
| 10 | 18-Mar-19 | Mon | 25 | | Interpolation |
| 10 | 19-Mar-19 | Tue | 26 | | Interpolation |
| 10 | 20-Mar-19 | Wed | 27 | | Interpolation |
| 10 | 21-Mar-19 | Thu | | | No class – Non-instructional day—Holi |
| 10 | 22-Mar-19 | Fri | | 11 | Non-linear equations |
| 11 | 25-Mar-19 | Mon | 28 | | Numerical Differentiation |
| 11 | 26-Mar-19 | Tue | | | Quiz II |
| 11 | 27-Mar-19 | Wed | 29 | | Numerical Differentiation |
| 11 | 28-Mar-19 | Thu | | 12 | Interpolation |
| 11 | 29-Mar-19 | Fri | | | |
| 12 | 1-Apr-19 | Mon | 30 | | Numerical Integration |
| 12 | 2-Apr-19 | Tue | 31 | | Numerical Integration |
| 12 | 3-Apr-19 | Wed | 32 | | Solving ODEs |
| 12 | 4-Apr-19 | Thu | | 13 | Numerical differentiation and integration |
| 12 | 5-Apr-19 | Fri | | | |
| 13 | 8-Apr-19 | Mon | 33 | | Solving ODEs |
| 13 | 9-Apr-19 | Tue | 34 | | Solving ODEs |
| 13 | 10-Apr-19 | Wed | 35 | | Solving ODEs |
| 13 | 11-Apr-19 | Thu | 36 | | Solving ODEs |
| 13 | 12-Apr-19 | Fri | | | |
| 14 | 15-Apr-19 | Mon | 37 | | Solving ODEs |
| 14 | 16-Apr-19 | Tue | 38 | | PDEs |
| 14 | 17-Apr-19 | Wed | | | Holiday – Mahavir Jayanti |
| 14 | 18-Apr-19 | Thu | | 14 | Solving ODEs |
| 14 | 19-Apr-19 | Fri | | | Holiday – Good Friday |
| 15 | 22-Apr-19 | Mon | 39 | | PDEs |
| 15 | 23-Apr-19 | Tue | | 15 | Solving ODEs |
| 15 | 24-Apr-19 | Wed | | 16 | Solving PDEs |
| 15 | 25-Apr-19 | Thu | 40 | | PDEs |
| 15 | 26-Apr-19 | Fri | | | |
| 16 | 30-Apr-19 | Tue | | | End Semester Examination |

Feedback

Any suggestions for improvement are welcome at any time. A mid-term feedback will happen on 11th February, 2019. The final feedback will happen during the TCF/registration week.

Reading

Books

- Heath MT (2002) *Scientific Computing*. The McGraw-Hill Companies, Inc., 2nd/e. ISBN 9781259002281
- Chapra S (2011) *Applied Numerical Methods W/MATLAB: for Engineers & Scientists*. McGraw-Hill Science/Engineering/Math, 3/e. ISBN 9781259027437

- Moler CB (2004) *Numerical Computing with Matlab*. Society for Industrial and Applied Mathematics. ISBN 9788120346819
- Press WH, Teukolsky SA, Vetterling WT, and Flannery BP (2007) *Numerical Recipes 3rd Edition: The Art of Scientific Computing*. Cambridge University Press, 3/e. ISBN 0521880688
- Mathews JH and Fink KK (2004) *Numerical Methods Using Matlab (4th Edition)*. Pearson, 4/e. ISBN 9788120327658

Last updated: January 15, 2019