

**QUALITY ASSURANCE MANUAL
DEPARTMENT OF BIOCHEMISTRY AND MICROBIOLOGY**

MSc PROGRAMME OUTLINE		
MSc in Bioinformatics and Computational Molecular Biology		
Course Work / Project Masters	Year: 2018	Coordinators: Prof Özlem TAŞTAN BISHOP & Dr Vuyani MOSES

COURSE WORK and RESEARCH THESIS MASTERS

in

**BIOINFORMATICS and
COMPUTATIONAL MOLECULAR BIOLOGY**

2018

DEPARTMENTS

of

**BIOCHEMISTRY & MICROBIOLOGY,
CHEMISTRY and STATISTICS**

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ORIENTATION

(8 February 2018, Thursday)

(Place: RUBi Seminar Room, 510, Biological Sciences Building 5th Floor)

14:00 – 14:30	Welcoming and introduction of RUBi members
14:30 – 15:00	Introduction to the programme
15:00 – 15:30	Introduction to plagiarism
15:30 – 16:30	Laptops will be given to the students who completed the registration process. Dr Vuyani Moses and Mr Olivier Sheik Amamuddy will be handing out the laptops to registered students

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PROPOSED PROGRAMME FOR 2017

Date	Module	Content
12 Feb , Mon - 16 Feb , Fri [25 contact hours]	Introduction to Linux Dr Rowan Hatherley	Linux operating system and software installation; Use of Linux and Linux shell commands; Introduction to Bash and Bash scripting; Application to Bioinformatics problems
19 Feb , Mon – 23 March , Fri [80 hours]	Python for Bioinformatics Dr Rowan Hatherley	Introductory and advanced Python; HPC cluster
26 March , Mon – 28 March , Wednesday 4 Apr , Wed – 6 April Fri [25 hours]	Basic Genomics Dr Vuyani Moses	Biological databases; Data retrieval; Sequence alignment and visualization
29 Apr , Fri – 17 Apr , Mon	Easter holiday	
9 Apr , Mon - 13 Apr , Fri [25 hours]	Structural Bioinformatics I Dr Vuyani Moses	Introduction to structural biology; Homology modeling and model validation
16 Apr , Mon - 20 Apr , Friday	Study/revision week	

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23 Apr, Mon – 26 Apr, Thu	EXAMINATIONS: <ul style="list-style-type: none"> • Linux (23 April) • Python (24 April) • Basic genomics (25 April) • Structural Bioinformatics (26 April) 	
2 May, Wed & 11 May, Fri 40 hours	Introduction to Mathematics and MATLAB Ms Caroline Ross	Review of basic calculus and linear algebra; Introduction to Normal Mode Analysis, constructing the Hessian Matrix, decomposition and the pseudoinverse of matrices using ProDy. Cross correlation studies and visualisation of respective modes The MATLAB computational environment, matrix manipulation, graphics. Writing efficient programs and functions.
14 May, Mon - 18 May, Fri [25 hours]	Structural Bioinformatics II Dr Kevin Lobb	Computational Chemistry Levels of theory. Protein-small molecule interactions; Autodock.
21 May, Mon - 25 May, Fri	Study/revision week	
28 May, Mon - 1 Jun, Fri [25 hours]	Statistics Mr Jeremy Baxter	Introductory statistics; R: statistical software
4 Jun, Mon - 8 Jun, Fri [25 hours]	Structural Bioinformatics III Dr Vuyani Moses	Force field parameter evaluation

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11 Jun, Mon - 15 Jun, Fri [25 hours]	Structural Bioinformatics IV Dr Vuyani Moses	Molecular Dynamics simulation of ligand protein interactions
18 Jun, Mon – 21 Jun Thr	Study/revision days	
	EXAMINATIONS: <ul style="list-style-type: none"> Mathematics (22 June) MATLAB (25 June) Structural Bioinformatics II (26 June) Statistics (27 June) Structural Bioinformatics III (28 June) Structural Bioinformatics IV (29 June) 	
2 July– 13 July	BREAK	
16 Jul, Monday	Project starts!	
23 Jul, Monday	PROJECTS: Hand-in Literature Review and Project Proposal to Supervisor and Co-supervisor – Project starts!	
Week of 30 Jul	PROJECTS: Project Proposal Presentations	
18 Jul, Wed – 21 Nov, Wed	BIOINFORMATICS JOURNAL CLUB	
Week of 3 Sep	1 st Presentation of Project Progress	
Week of 15 Oct	2 nd Presentation of Project Progress	
Week of 26 Nov	Presentation of project results	
10-14 Dec	Thesis submission (If thesis on time)	

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OVERALL TEACHING HOURS

	Contact Hours	Lecturing Hours	Practicals and tutorials
Introduction to Linux	25	10	15
Python for Bioinformatics	80	32	48
Basic Genomics	25	10	15
Structural Bioinformatics I	25	10	15
Mathematics	25	10	15
MATLAB	25	10	15
Structural Bioinformatics II	25	10	15
Statistics	25	10	15
Structural Bioinformatics III	25	10	15
Data structures and algorithm development	25	10	15
TOTAL	305	122	183

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COURSE OUTCOMES

CRITICAL OUTCOMES ADDRESSED

1. Identify and solve problems and make decisions using critical and creative thinking
2. Work effectively with others as a team
3. Organise and manage time and activities effectively
4. Collect, analyse, organise, and critically evaluate information
5. Communicate effectively using written, electronic and language skills
6. Use science and technology effectively and critically showing responsibility towards the environment and others
7. Demonstrate an understanding of the world as a set of related systems

SPECIFIC OUTCOMES ADDRESSED:

1. Develop a broad understanding of what the field of Bioinformatics and Computational Molecular Biology comprises
2. Develop an in-depth knowledge of certain major areas of Bioinformatics and Computational Molecular Biology
3. Demonstrate the ability to conduct research by designing and carrying out a piece of research in Bioinformatics and Computational Molecular Biology, including design of computational experiments and collection and analysis of data
4. Demonstrate expertise in scientific writing, oral presentation and communication
5. Demonstrate an understanding of the relationship between Bioinformatics and Computational Molecular Biology, the community and the environment
6. Demonstrate the competence required for recognition as a professional Bioinformaticist or Computational Molecular Biologist in South Africa
7. Develop professional attitudes and values including scientific ethics and integrity

PARTICULAR SKILLS TO BE ACQUIRED:

1. Scientific communication and presentation skills including computer skills
2. Ability to use the scientific literature efficiently and effectively
3. Practical skills required for use and application of computers and software
4. Organisational skills required to acquire, manage and utilise data and information
5. Ability to analyse and evaluate scientific data
6. Good computer practice

GENERAL BACKGROUND & OUTCOMES

Bioinformatics and computational molecular biology is the systematic development and application of information technologies and data mining techniques for analysing biological data obtained by experiments, modelling, database searching and instrumentation to make novel observations and predictions about biological function. This course will be taught in an interdisciplinary manner and focussing on the interface between the computational sciences and the biological, physical and chemical sciences. Graduates who complete this course will

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be skilled in the assimilation of biological information through the use and development of computational tools for a range of applications including simple pattern recognition, molecular modelling for the prediction of structure and function, gene discovery and drug target discovery, the analysis of phylogenetic relationships, whole genome analysis and the comparison of genetic organization.

COURSE STRUCTURE, TEACHING METHODS & APPROACH

The Masters programme will be offered over 11 months and incorporate a number of course work modules and a research project running concurrently throughout the programme. The course work modules will involve an integration of formal lectures, self-learning computer-based tutorials and practicals. In addition, problem solving tutorials would be designed to guide the student through current information-based problems and involve the assimilation and reduction of biological information. A number of the tutorials and practical components will be assessed and contribute towards a course work year mark. The assessment of the course work component would be through assignments, tutorials, tests etc., and examinations. Each examination will have an external examiner, appointed by the lecturer's home Department (for lecturers from Rhodes), or by the Department of Biochemistry, Biotechnology and Microbiology (for external lecturers).

The research projects will be computer based. The projects will be assessed by seminar presentations of the proposed and final work, and by a written thesis. Each thesis will be examined by two external examiners.

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ASSESSMENT

OVERALL

The course-work and the research work will each contribute 50% to an overall mark. Successful completion of the course will be subject to a final mark of at least 50%, provided that a candidate obtains at least 50% for the course work, with a sub-minimum of at least 40% from each module, and at least 50% for the project report.

COURSE WORK

The course-work modules will be assessed by internal grading of tutorials, assignments, tests and practicals, etc. to give a class mark; and by internal and external grading of examinations. The calculation of the class mark for each module is given later in this manual under the detailed entry for the module. The examinations will be given during the period specified in the course programme earlier in this manual. For each module, the weighting between class mark and examination towards the module mark will be

- Class mark 40%
- Examinations 60%

The weightings of the various modules in the calculation of the overall course work mark will be proportional to the number of lectures given. For each module the weighting, and the duration of the examination, will be

Module	Weighting	Duration (hours – up to)
Introduction to Linux	8.2%	3
Python for Bioinformatics	26.2%	4-5
Basic Genomics	8.2%	3
Structural Bioinformatics I	8.2%	3
Mathematics	8.2%	3
MATLAB	8.2%	3
Structural Bioinformatics II	8.2%	3
Statistics	8.2%	3
Structural Bioinformatics III	8.2%	3
Data structures & algorithm	8.2%	3

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PROJECT

The project will be graded internally and externally with the following weightings:

- | | |
|-------------------------------------|-----|
| • Project proposal and presentation | 10% |
| • Project results and presentations | 30% |
| • Thesis | 60% |

PROPOSAL:

Guidelines

Preparation for the Research Project Proposal (written and oral) should be commenced as soon as the projects have been allocated.

Written

Style: Follow the style of any journal article on Bioinformatics

Length: Around 20 typed pages. Include sections on: Literature review (around 15 pgs); problem statement and hypothesis (1 pg); aims and objectives (1 page); outline of approach and methodology (1–2 pgs).

References: Follow the citation and listing style of the journal, (references may be single-spaced).

Oral

Length: 30 minutes; 25 minutes presentation and 5 minutes questions.

Dates

As specified in the programme earlier in this manual.

Marks Breakdown

- | | |
|--------------------------|-----|
| • Proposal presentation: | 50% |
| • Written proposal: | 50% |

PRESENTATION OF PROJECT RESULTS:

Guidelines

The Research Project Results presentation should include:

- **Introduction** - an explanation of the background to the project, the current status of the scientific field, a clear hypothesis statement, and the overall aims & objectives of the project.
- **Description of the approach**, the techniques and methodology, including reasons for why these computations were done.

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- **Presentation and Explanation of Results.**
- **Critical discussion of results** including analysis of their implications, and any problem areas.
- **Conclusion** that includes the overall outcome of the project and where future research should be directed.

Dates

As specified in the programme earlier in this manual.

THESIS:

Structure

There is some flexibility in the choice of format for a thesis, but as a guide, it should contain the following sections in the order given:

- Abstract
- Table of Contents
- Table of Figures
- List of Tables
- List of Abbreviations
- Acknowledgements
- Chapters 1 (Literature review)
- Chapter 2, 3, etc
- Conclusion
- References

Each Chapter following Chapter 1 would normally contain

- Introduction
- Methods
- Results and Discussion

Dates

As specified in the programme earlier in this manual.

ASSESSMENT CRITERIA & PROCEDURE

The thesis will be assessed by two external examiners. Preferably, at least one of the external examiners should be international.

NUMBER OF COPIES OF THE RESEARCH REPORT

You should prepare two copies of your thesis for external examiners. After corrections are done, one final copy should be prepared for RUBi.

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DESCRIPTION OF THE MAJOR SECTIONS OF THE THESIS

1. ABSTRACT

An abstract has to stand alone and should: (i) state the principal objectives and scope of the investigation; (ii) state the methodology used; (iii) summarize the results; (iv) state the principal conclusions. It should not exceed a page.

2. CHAPTER 1

Literature review

This should be a concise summary that describes the current status of the research field. It should be current and comprehensive.

Project aims, objectives and motivation

A clear statement of the aims & objectives of the project and motivation for these should be given. Knowledge gap should be explained.

3. FURTHER CHAPTERS

Introduction

This should be a concise summary that describes the current status of the literature related to the chapter.

Methodology

This should give a logical account of the methodology. It should be precise and complete.

Results and Conclusion

This section should give a description of the results of the experiments together with an explanation of why they were done. It should include critical analysis of the data and interpretation of the implications of the results.

5. CONCLUSION

Should be a concise and relevant summary, including the contribution the research makes to the current status of the field. A statement of the direction of future research arising from the project should be given.

6. REFERENCES

Current research articles should be used and cited in the text of the thesis using the style of a bioinformatics journal.

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EVALUATION FORMS

MSc Proposal Presentation Evaluation Criteria

Criterion	Weight
1. Concise, accurate & up-to-date literature review	20
2. Knowledge gap and/or problem clearly identified and stated	20
3. Clear research hypothesis & objectives; Concise description of approach and methods	20
4. Research objectives, approach & methods. Realistic? Feasible?	15
5. Time management, visual media and speaker – audience contact	10
6. Ability of speaker to answer questions in a clear & meaningful manner.	15

MSc Written Proposal Evaluation Form

Criterion	Weight
1. Concise, accurate & up-to-date literature review	30
2. Knowledge gap and/or problem clearly identified and stated	20
3. Clear research hypothesis & objectives; Concise description of approach and methods	20
4. Research objectives, approach & methods. Realistic? Feasible?	15
5. Quality of scientific writing	15

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MSc Project Progress Presentation Evaluation Criteria

Criterion	Weight
1. Clear research hypothesis & objectives	10
2. Concise description of approach and methods	15
3. Results and discussion: interpretation of results and critical analysis of their meaning and impact	45
4. Summary of findings and future plans	10
5. Ability of speaker to answer questions in a clear & meaningful manner.	10
6. Time management, visual media and speaker – audience contact	10

MSc Final Project Presentation Evaluation Criteria

Criterion	Weight
1. Concise, accurate & up-to-date literature review	15
2. Knowledge gap and/or problem clearly identified and stated	15
3. Clear research hypothesis & objectives; Concise description of approach and methods	15
4. Results and discussion: interpretation of results and critical analysis of their meaning and impact	25
5. Summary of findings and future plans	5
6. Time management, visual media and speaker – audience contact	10
7. Ability of speaker to answer questions in a clear & meaningful manner.	15

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PLAGIARISM

Plagiarism is a serious offence. All students are expected to familiarize themselves with the Rhodes University Policy on Plagiarism:
<https://www.ru.ac.za/media/rhodesuniversity/content/institutionalplanning/documents/Plagiarism.pdf>

Before lectures start, each student must sign the plagiarism declaration page and return to the course coordinator.

It is important to understand that in a senior course, a first offence is taken more seriously than in an introductory course.

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Student Name:

Student No:

PLAGIARISM DECLARATION FORM

1. I am aware of and I have familiarized myself with the Rhodes University Policy on Plagiarism:
<https://www.ru.ac.za/media/rhodesuniversity/content/institutionalplanning/documents/Plagiarism.pdf>
2. I know that “plagiarism” means using another person’s work and ideas without acknowledgement, and pretending that it is one’s own. I know that plagiarism not only includes verbatim copying, but also the extensive (albeit paraphrased) use of another person’s ideas without acknowledgement. I know that plagiarism covers this sort of use of material found in theses, textbooks, journal articles AND on the internet.
3. I acknowledge and understand that plagiarism is wrong, and that it constitutes academic theft.
4. I understand that my research must be accurately referenced.
5. All the assignments that I submit during my MSc degree are my own work, or the unique work of a group, if a group assignment.
6. I have not allowed, nor will I in the future allow, anyone to copy my work with the intention of passing it off as his or her own work. I also accept that submitting identical work to someone else (a syndicate essay) constitutes a form of plagiarism.

Signed _____

Date _____

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COURSE WORK MODULES

INTRODUCTION TO LINUX

Lecturer: Dr Rowan Hatherley

Contact hours: 25

SPECIFIC OUTCOMES ADDRESSED

1. To be able to install a Linux operating system
2. Work comfortably and proficiently in Linux
3. To be able to install and use software in Linux
4. Master several shell commands

BACKGROUND KNOWLEDGE REQUIRED

Basic computer literacy: proficiency with word-processing, spreadsheets and graphics programs, exposure to standard bench-top computational tools and the web

TEACHING METHODS/APPROACH

The lectures will be complemented by tutorials and self-study

BOOKS & OTHER SOURCES USED

An Introduction to the Linux Command Shell for Beginners by Victor Gedris
GNU/Linux Command-Line Tools Summary by Gareth Anderson
Introduction to Linux – A Hand on Guide by Machtelt Garrels

COURSE CONTENT

1. Overview of Linux
2. Linux installation
3. Basic commands
4. The Linux file system
5. Working with files and folders in Linux
6. I/O redirection
7. Networking and connecting to an external server
8. Fundamental backup systems
9. Software management
10. Overview of Bash and Bash scripting
11. Miscellaneous advanced

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

1. Daily exercises and assignments: 60%
2. Test 1: 40%

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PYTHON FOR BIOINFORMATICS

Lecturers: Dr Rowan Hatherley

Contact hours: 80

SPECIFIC OUTCOMES ADDRESSED

1. To understand what programming is and why it is useful/necessary
2. To become familiar with the different variable types and data structures available in Python
3. To be able to write Python programs to solve basic problems
4. To be able to section off useful bits of code into Python functions
5. To understand and implement object-orientated programming
6. Advance string handling
7. Reading and writing files
8. Useful modules and libraries (os, sys, numpy, scipy, pymol, args) and how to use them
9. Biological data analysis using Python
10. Handle errors efficiently and elegantly
11. Design and build command line tools with Python that adhere to best practices
12. Understand how to use an HPC cluster and submit jobs in a high throughput fashion

BACKGROUND KNOWLEDGE REQUIRED

Basic computer literacy; Basic understanding of the Linux operating system; Understanding of system directories

TEACHING METHODS/APPROACH

Teaching will consist of lectures and numerous small exercises and assignments to allow students to learn from practical experience

BOOKS & OTHER SOURCES USED

Python documentation: <http://docs.python.org/index.html>

COURSE CONTENT

1. Introduction to Python and simple commands
2. Conditionals and loops
3. Data structures
4. Functions
5. Classes and objects
6. Files
7. Regular expressions
8. String handling
9. Useful modules in Python
10. Scripting job submission to a cluster with Python

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- 11. Error handling
- 12. Tips and tricks

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

- 1. Daily exercises and assignments: 40%
- 2. Test: 20%
- 3. Project: 40%

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BASIC GENOMICS

Lecturer: Dr Rowan Hatherley

Contact hours: 25

SPECIFIC OUTCOMES ADDRESSED

1. Become familiar with biological databases
2. Ability to retrieve and analyse data from biological databases
3. Understand various alignment algorithms
4. To be able to align homologous sequences in DNA or protein format and understand the advantages and disadvantages of the two approaches

BACKGROUND KNOWLEDGE REQUIRED

Basic biochemistry and genetics knowledge

TEACHING METHODS/APPROACH

The lectures will be complemented by tutorials, self-study and article discussions

BOOKS & OTHER SOURCES USED

1. Essential Bioinformatics by Jin Xiong
2. Bioinformatics – A practical guide to the analysis of genes and proteins by Andreas Baxevanis and Francis Ouellette
3. Manuals and tutorials of various sequence alignment programs
4. Research articles

COURSE CONTENT

1. Biological databases
2. Homology detection programs
3. Sequence alignment
 - a. Pairwise sequence alignment
 - b. Multiple sequence alignment
 - c. Profiles and HMMs
4. Sequence visualization programs

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

1. Daily assignments 40%
2. Small project: 30%
3. Test: 30%

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STRUCTURAL BIOINFORMATICS – I

Lecturer: Dr Rowan Hatherley

Contact hours: 25

SPECIFIC OUTCOMES ADDRESSED

1. To understand structural biology terminology, especially X-ray crystallography
2. To learn how to use different protein visualization programs
3. To understand various secondary and tertiary structure prediction algorithms
4. To understand the range, applications and limitations of modeling methods
5. To learn and understand the various steps involved in homology modeling
6. To learn homology modeling using Modeller
7. To be able to use different model evaluation programs and understand how they work

BACKGROUND KNOWLEDGE REQUIRED

1. Knowledge on biochemical properties of amino acids
2. Basic understanding of primary, secondary, tertiary and quaternary protein structure
3. Knowledge on non-covalent bond formations

TEACHING METHODS/APPROACH

The lectures will be complemented by tutorials, self-study and article discussions

BOOKS & OTHER SOURCES USED

1. Essential Bioinformatics by Jin Xiong
2. Bioinformatics – A practical guide to the analysis of genes and proteins by Andreas Baxevanis and Francis Ouellette
3. Molecular Modeling and Simulation - An Interdisciplinary Guide by Tamar Schlick
4. Manuals and tutorials of various modeling and visualization programs

COURSE CONTENT

1. Structural biology techniques
2. The Protein Data Bank
3. Protein visualization programs
4. Protein secondary and tertiary structure prediction
5. Homology modeling with Modeller
6. Model validation programs

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

- | | |
|----------------------|-----|
| 1. Daily assignments | 40% |
| 2. Small project: | 30% |
| 3. Test: | 30% |

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BASIC MATHEMATICS

Lecturer: Ms Caroline Ross

Contact hours: 25

SPECIFIC OUTCOMES ADDRESSED

1. Acquire background knowledge of calculus and linear algebra for Matlab course
2. Use linear algebra to investigate the motions of a protein structure through Normal Mode Analysis
3. Use the python package for Normal Mode Analysis of proteins. In particular the following steps will be included:
 - a. Construction of Hessian Matrix
 - b. Matrix Decomposition to obtain eigenvectors and eigenvalues of each mode
 - c. Calculation of Covariance Matrix
 - d. Alternate and understand the cutoff range
4. Understand and develop the ability to code the algorithms presented in the ProDy package.
5. Visualise respective modes of proteins in VMD

BACKGROUND KNOWLEDGE REQUIRED

Basic calculus, algebra, linear algebra, protein structures

TEACHING METHODS/APPROACH

The lectures will be complemented by self-study and tutorials.

BOOKS & OTHER SOURCES USED

Lecture notes

Any Calculus, Linear Algebra books

COURSE CONTENT

1. Calculus (Differentiation and integration)
2. Linear Algebra (Matrices, eigenvalue / eigenvector problems)
3. Normal Mode Analysis (ProDy, construction of the hessian matrix, decomposition packages, cross correlation studies and visulisation of modes in VMD)

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

1. Test (Calculus and Linear Algebra): 40%
2. Assignment (Normal Mode Analysis): 60%

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MATLAB AND NEURAL NETWORKS

Lecturer: Prof Nigel Bishop

Contact hours: 25

SPECIFIC OUTCOMES ADDRESSED

1. Use of the MATLAB computational environment.
2. Write programs and scripts in the MATLAB language to solve problems.
In particular, use MATLAB to:
 - set up a mathematical model for a physical/chemical/biological system
 - solve a system of linear equations
 - solve a system of non-linear equations
 - solve a system of non-linear differential equations
3. Construct, train and deploy artificial neural networks to solve a variety of scientific problems.

BACKGROUND KNOWLEDGE REQUIRED

1. Calculus of functions of several variables. In particular:
 - derivatives and partial derivatives
 - tangent lines and planes
 - the integral of a function of one variable
2. Linear algebra: matrix algebra

TEACHING METHODS/APPROACH

Lectures and structured exercises.

BOOKS & OTHER SOURCES USED

Notes will be provided.

COURSE CONTENT

The MATLAB environment

MATLAB programs and functions

Solving linear and non-linear systems of equations and differential equations with MATLAB

Artificial Neural Networks with MATLAB

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

Assignments: 50%

Test: 50%

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STRUCTURAL BIOINFORMATICS – II

Lecturer: Dr. Kevin A. Lobb

Contact hours: 25

SPECIFIC OUTCOMES ADDRESSED

This course introduces the theory and practice of molecular modelling as used in chemistry and medicinal chemistry. Although competence in the use of several software packages is a critical component, emphasis will be on the understanding of the methods and on strategies in their application to a wide variety of problems.

BACKGROUND KNOWLEDGE REQUIRED

Little background knowledge is required, beyond that of basic chemistry. However it is essential that you are comfortable with chemical structures and that you can quickly identify whether they are correct or incorrect in terms of positioning and the valency of atoms. Familiarity with the any following concepts would be helpful, though not essential as we will deal with what is necessary during the course. Conformational analysis (e.g. boat and chair cyclohexane); orbitals, HOMO, LUMO, bonding and antibonding, excited state; Infrared Spectroscopy; transition state; activation energy; enthalpy, entropy and free energy.

TEACHING METHODS/APPROACH

The teaching will be split equally between lectures and practicals.

BOOKS & OTHER SOURCES USED

User manuals and background from the programs Materials studio, Gaussian, CHARMM, GAMESS, VASP, Autodock, Vega ZZ, CPMD, Sparky and relevant supplied journal articles.

COURSE CONTENT

Theories used in calculations, molecular mechanics, semi-empirical, Hartree-Fock, configuration interaction and density functional theory. Correlation energy. Basis sets. Strategies for dealing with extremely large systems. Combined methods QM/MM, ONIOM, discrete and continuum solvation. Exploring the potential energy surface and vibrational analysis. Conformational searches. Calculable properties. Excited states. Calculations in vacuo, periodic boundary conditions.

Chemical Libraries. Molecular docking – construction of small molecules, preparation of protein and the docking procedure. Docking via scripting, and high-throughput virtual screening.

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

There will be an assignment which will make up 100% of the mark for this course.

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INTRODUCTORY STATISTICS

Lecturer: Mr. Jeremy Baxter

Contact hours: 25

SPECIFIC OUTCOMES ADDRESSED

The aims of this course are:

1. To provide students with the basics of probability theory (probability, probability axioms, conditional probability, probability density function, cumulative distribution function, expectation, variance, discrete random variable, continuous random variable) and statistical background, concepts and techniques (statistical experiment, descriptive statistics, inference statistics) that are most useful to Bioinformaticians.

On completion of the course students should, inter alia, be able to:

1. Explain the differences between a population and a sample.
2. Collect, summarise and describe data using suitable numerical and graphical techniques.
3. Explain the concepts of probability, interpret probabilities and use suitable theory to calculate simple and conditional probabilities.
4. Identify discrete and continuous probability distributions.
5. Demonstrate the use of the binomial, Poisson, normal, Student t, chi-square and F distributions.
6. Calculate point and interval estimates, one- and two-sample, for the population mean(s), proportion(s) and variance(s) and interpret the meaning of each.
7. Perform suitable hypothesis tests (parametric and or non-parametric procedure) for one- and two-sample analyses and draw meaningful conclusions and decisions for the population mean(s), proportion(s) and variance(s).
8. Estimate, interpret and make predictions using linear models. Perform suitable statistical inference and model diagnostics for linear models.

BACKGROUND KNOWLEDGE REQUIRED

1. Basic Calculus: Differentiation and integration
2. Linear algebra: Matrices, vectors
3. Matlab literacy, specifically matrix operations.
4. Basic programming experience, in python or perl

TEACHING METHODS/APPROACH

This course will be taught using formal lectures, typically in the morning, and self-study tutorials and practicals. Use of hand-outs, notes, text books, board-work and overheads. Relevant notions from linear algebra and statistics will be discussed and the student will then be required to read portions of prescribed texts on his/her own. At each lecture a set of exercises will be presented and completed ready for assessment by the next lecture.

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BOOKS & OTHER SOURCES USED

1. J Baxter, Introductory Statistics for Bioinformaticians using R (course notes/slides).
2. Wim P. Krijnen, 2009, Applied Statistics for Bioinformatics using R, CRAN

COURSE CONTENT

1. A brief introduction to R.
2. Descriptive statistics (Graphical and numerical summaries of univariate, bivariate and multivariate data).
3. An introduction to statistical distributions.
4. Estimation and inference for one/ two random samples (Parametric and non parametric methods.)
5. An introduction to correlation, linear regression and linear models: (One and Two Way ANOVA)

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

1. Daily assignments/exercises: 40%
2. Tests: 60%

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STRUCTURAL BIOINFORMATICS – III

Lecturer: Mr Vuyani Moses

Contact hours: 25

SPECIFIC OUTCOMES ADDRESSED

This course will introduce the principle of molecular dynamics (MD) simulations to study protein-ligand interactions. This will require the docked protein-ligand complex that would have been generated in the “STRUCTURAL BIOINFORMATICS II” course. In cases where there are no force field parameters for part of the system to be simulated, force field parameters may be generated by QM/MM studies. As a result, part of this course will focus on generating force field parameters for metal containing systems.

BACKGROUND KNOWLEDGE REQUIRED

This course will require basic understanding of protein systems, in particular protein-ligand complexes and metal containing enzymes interactions.

TEACHING METHODS/APPROACH

This course will be a combination lectures and practicals/tutorials

BOOKS & OTHER SOURCES USED

Reading the user manuals and the tutorials of the programs to be used will be advantageous. The programs to be used are:

CHARMM
GROMACS
Gaussian09

COURSE CONTENT

1. The principles of Molecular dynamics simulations of protein-ligand complexes (in GROMACS).
 - i. Structure preparation
 - ii. Solvation
 - iii. Neutralization
 - iv. energy minimization
 - v. Equilibration
2. Trajectory analysis:
 - i. Root Mean Square Deviation
 - ii. Radius of gyration
 - iii. Potential energy
 - iv. Visualization in VMD
3. Force field parameter generation
 - i. QM/MM potential energy surface scans (PES) (in Gaussian09)

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- ii. List squares fitting to generate force field parameters
- iii. MD simulations to validate force field parameters (in CHARMM)

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

A single assignment will to assess the course. This assignment will represent 100% of the course mark.

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DATA STRUCTURES AND ALGORITHM DEVELOPMENT

Lecturer: Prof Philip Machanick

Contact hours: 25

SPECIFIC OUTCOMES ADDRESSED

The aims of this course are to provide students with the basics of algorithm and memory usage analysis focused on the needs of Bioinformaticians.

On completion of the course students should, inter alia, be able to:

1. Explain the differences between space and time complexity.
2. Understand how an algorithm scales up with increased data based on its complexity class.
3. Explain the concepts of divide and conquer, greedy and dynamic programming algorithms.
4. Demonstrate ability to construct algorithms and data structures from scratch and to know when to use built in algorithms and data structures in a given language.
5. Demonstrate ability to implement and apply known algorithms, particular as apply to Bioinformatics.
6. Perform analysis of a given algorithm or data structure.
7. Know common algorithms used in Bioinformatics in areas such as sequence alignment, clustering, motifs (finding and searching).

BACKGROUND KNOWLEDGE REQUIRED

1. Programming in Python and familiarity with the Linux command line.
2. Ability to prove results in discrete mathematics particularly proof by induction.
3. Understanding of common applications of bioinformatics.

TEACHING METHODS/APPROACH

The course is taught using the “Flipped Classroom” strategy. Class members are expected to be up to date with material prior to discussion. Instead of teaching you then having you go away and do homework, you are expected to understand the basics and bring your homework to class to discuss how to complete it.

BOOKS & OTHER SOURCES USED

General algorithms reference; remaining materials online:

Thomas H. Cormen, Charles E. Leiserson, Ronald L. Rivest, and Clifford Stein. *Introduction to Algorithms* (3rd ed.), MIT Press, 2009

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COURSE CONTENT

1. Applicable mathematical methods
2. Complexity classes – time and space and basics of analysis
3. Algorithm design approaches – divide and conquer, greedy, dynamic programming, heuristics
4. Common data structures algorithms – general and bioinformatics
5. Built-in languages features vs. code from scratch

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

Assessment by assignment 60% and test 40%.

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