

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

MSc PROGRAMME OUTLINE

MSc in Bioinformatics and Computational Molecular Biology

Course Work / Project Masters	Year: 2016	Coordinator: Prof Özlem TAŞTAN BISHOP
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COURSE WORK and RESEARCH THESIS MASTERS

in

**BIOINFORMATICS and
COMPUTATIONAL MOLECULAR BIOLOGY**

2016

DEPARTMENTS

of

**BIOCHEMISTRY & MICROBIOLOGY,
CHEMISTRY, MATHEMATICS and STATISTICS**

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ORIENTATION

(15 February 2016, Monday)

(Place: Biochemistry Seminar Room 1, Biological Sciences Building 5th Floor)

14:00 – 14:30	Welcoming and introduction of RUBi members
14:30 – 15:30	“Introduction to the programme” by Prof Özlem Taştan Bishop
15:30 – 16:30	Laptops will be given to the students who completed the registration process (RUBi Lab 129A)

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PROPOSED PROGRAMME FOR 2016

Date	Module	Content
16 Feb , Tue - 19 Feb , Fri [20 contact hours]	Introduction to Linux Prof Özlem Taştan Bishop	<ul style="list-style-type: none"> • Linux operating system and software installation • Use of Linux and Linux shell commands • Application to Bioinformatics problems
22 Feb , Mon – 26 Feb , Fri [25 hours]	Basic Genomics Prof Özlem Taştan Bishop	DNA and protein databases; database searching; sequence alignment
29 Feb , Mon – 1 April , Fri [75 hours]	Python for Bioinformatics Dr Rowan Hatherley, Mr David Penkler Mr David Brown	<ul style="list-style-type: none"> • Introductory and advanced Python • HPC cluster
25 Mar , Fri – 28 Mar , Mon	Easter holiday	
4 Apr , Mon – 8 Apr , Friday 15 hours	Introduction to Mathematics Prof Özlem Taştan Bishop	Review of basic calculus and linear algebra
11 Apr , Mon - 15 Apr , Fri [25 hours]	Structural Bioinformatics I Prof Özlem Taştan Bishop	Homology modeling and model validation

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18 Apr, Mon - 22 Apr, Fri	Study week	
25 Apr, Mon – 29 Apr, Fri	EXAMINATIONS: <ul style="list-style-type: none"> • Linux (25 April) • Basic genomics (26 April) • Basic mathematics (25 April) • Python (28 May) • Structural Bioinformatics (29 April) 	
3 May, Tue – 13 May, Fri [40 hours]	MATLAB and Neural Networks Prof Mike Burton	<p>The MATLAB computational environment, matrix manipulation, graphics. Writing efficient programs and functions.</p> <p>Constructing and deploying artificial neural networks for prediction, interpolation and pattern recognition. Examples from physics, economics, chemistry, biochemistry, biotechnology, medicine, biology.</p>
16 May, Mon - 20 May, Fri [25 hours]	Structural Bioinformatics II Dr Kevin Lobb Mr Thommas Musyoka	<p>Molecular dynamics; protein-small molecule interactions; Autodock.</p>
23 May, Mon - 27 May, Fri	Study week	
30 May, Mon - 3 Jun, Fri [25 hours]	Statistics Mr Jeremy Baxter	<p>Introductory statistics; R: statistical software</p>

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<p>6 Jun, Mon - 10 Jun, Fri</p> <p>[25 hours]</p>	<p>Metagenomics</p> <p>Prof Oleg Reva</p>	<ul style="list-style-type: none"> • Aims and techniques; • Next Generation Sequencing (NGS) for metagenomics; • Metabarcoding; • The most useful tools and Web-resources for metagenomics;
<p>13 June, Mon – 17 June, Fri</p>	<p>Study week</p>	
<p>20 Jun, Mon – 23 Jun, Thu</p>	<p>EXAMINATIONS:</p> <ul style="list-style-type: none"> • MATLAB and Neural Network (20 June) • Structural Bioinformatics II (21 June) • Statistics (22 June) • Metagenomics (23 June) 	
<p>24 Jun, Friday – 10 Jul, Sun</p>	<p>BREAK</p>	
<p>15 Jul, Friday</p>	<p>PROJECTS: Hand-in Literature Review and Project Proposal to Supervisor and Co-supervisor – Project starts!</p>	
<p>Week of 18 Jul</p>	<p>PROJECTS: Project Proposal Presentations</p>	
<p>27 Jul, Wed – 16 Nov, Wed</p>	<p>BIOINFORMATICS JOURNAL CLUB</p>	
<p>Week of 19 Sep</p>	<p>1st Presentation of Project Progress</p>	
<p>Week of 17 Oct</p>	<p>2nd Presentation of Project Progress</p>	
<p>Week of 28 Nov</p>	<p>Presentation of project results</p>	
<p>7-14 Dec</p>	<p>Thesis submission (If thesis on time)</p>	

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OVERALL TEACHING HOURS

	Contact Hours	Lecturing Hours	Practicals and tutorials
Introduction to Linux	20	8	12
Basic Genomics	25	12	13
Python for Bioinformatics	75	30	45
Introduction to Mathematics	15	8	7
Structural Bioinformatics I	25	11	14
MATLAB and Neural Network	40	15	25
Structural Bioinformatics II	25	11	14
Statistics	25	10	15
Metagenomics	25	11	14
TOTAL	275	116	159

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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 be skilled in the assimilation of biological information through the use and development of

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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)
Introduction to Linux	7.3 %	2
Basic Genomics	9.1 %	3
Python for Bioinformatics	27.2%	4-5
Mathematics	5.5%	2
Structural Bioinformatics I	9.1 %	3
MATLAB and Neural Network	14.5 %	3
Structural Bioinformatics II	9.1 %	3
Statistics	9.1 %	3
Metagenomics	9.1 %	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.
- **Presentation and Explanation of Results.**

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- **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:

http://www.ru.ac.za/static/policies/plagiarism_policy.pdf

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

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Student Name:

Student No:

PLAGIARISM DECLARATION FORM

1. I am aware of Rhodes University Policy on Plagiarism webpage and I have familiarized myself (http://www.ru.ac.za/static/policies/plagiarism_policy.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: Prof Özlem Taştan Bishop

Contact hours: 20

SPECIFIC OUTCOMES ADDRESSED

1. To be able to install a Linux operating system
2. To be able to install various programs
3. Log in and out of a Linux system
4. Work with directories and files and change file permissions
5. Master several shell commands
6. Redirect input and output and print documents

BACKGROUND KNOWLEDGE REQUIRED

Basic computer literacy: proficiency with word-processing, spreadsheets and graphics programmes, 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

Introduction to Linux – A Hand on Guide by Machtelt Garrels (tldp.org/LDP/intro-linux/intro-linux.pdf)

COURSE CONTENT

1. What is Linux?
2. How to install an operating system
3. Quick start
4. About files and file systems
5. Processes
6. I/O redirection
7. Text editors
8. Home
9. Printers and printing
10. Fundamental backup systems
11. Networking
12. Installation of various programs

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

1. Test 1: 100%

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BASIC GENOMICS

Lecturer: Prof Özlem Taştan Bishop

Contact hours: 25

SPECIFIC OUTCOMES ADDRESSED

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

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. Introduction to bioinformatics by Anna Tramontano
3. Bioinformatics – A practical guide to the analysis of genes and proteins by Andreas Baxevanis and Francis Ouellette
4. Research articles and other bioinformatics books in the library

COURSE CONTENT

1. Biological databases
2. Sequence alignment
 - a. Pairwise sequence alignment
 - b. Database similarity search
 - c. Multiple sequence alignment
 - d. Profiles and HMMs

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

1. Small project: 50%
2. Test: 50%

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PYTHON FOR BIOINFORMATICS

Lecturers: Dr Rowan Hatherly, Mr David Penkler, Mr David Brown

Contact hours: 75

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
11. Error handling

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12. Tips and tricks

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

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

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BASIC MATHEMATICS

Lecturer: Prof Özlem Taştan Bishop

Contact hours: 15

SPECIFIC OUTCOMES ADDRESSED

1. Describe biological/bioinformatics problems using mathematics.
2. Solve these problems using calculus, linear algebra.
3. Acquire background for Matlab and Statistics courses

BACKGROUND KNOWLEDGE REQUIRED

Basic calculus, algebra, linear algebra

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)

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

1. Test: 100%

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STRUCTURAL BIOINFORMATICS – I

Lecturer: Prof Özlem Taştan Bishop

Contact hours: 25

SPECIFIC OUTCOMES ADDRESSED

1. To understand structural biology terminology, especially X-ray crystallography, and to be able to follow the literature
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 modeling by using Modeller

BACKGROUND KNOWLEDGE REQUIRED

1. Knowledge on biochemical properties of amino acids
2. Basic understanding of the primary, secondary, tertiary and quaternary structure of proteins.
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. Introduction to bioinformatics by Anna Tramontano
3. Bioinformatics – A practical guide to the analysis of genes and proteins by Andreas Baxeavanis and Francis Ouellette
4. Manuals and tutorials of various modeling and visualization programs

COURSE CONTENT

1. Structural biology techniques
2. Protein visualization programs
3. Protein secondary structure prediction
4. Protein tertiary structure prediction
5. Homology modeling; Modeller

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

1. Short project: 50%
2. Test: 50%

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MATLAB AND NEURAL NETWORKS

Lecturer: Prof Mike Burton

Contact hours: 40

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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DEPARTMENT OF BIOCHEMISTRY AND MICROBIOLOGY**

MSc PROGRAMME OUTLINE

MSc in Bioinformatics and Computational Molecular Biology

Course Work / Project Masters

Year: 2016

Coordinator: Prof Özlem TAŞTAN BISHOP

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. Molecular dynamics (MM, Born-Oppenheimer and Car-Parrinello). Interaction between systems – basis set superposition error, protein-small molecule interactions and docking. NMR – relaxation, coupling and relevant experiments used in biomolecular NMR. Principles of structure assignment. Protein-ligand interactions by NMR.

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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METAGENOMICS

Lecturer: Prof Oleg Reva

Contact hours: 25

SPECIFIC OUTCOMES ADDRESSED

- Understanding of the theoretical background, principals, aims and techniques of metagenomics. Students will get knowledge regarding the areas of applicability of metagenomics and about associated limitations and possible artefacts of metagenomics.
- Ability to select the appropriate sequencing techniques to complete a metagenomics project. Students will get knowledge about different Next Generation Sequencing (NGS) approaches and their applicability in metagenomics. WGS and amplicon based metagenomic sequencing approaches will be compared.
- Students will gain knowledge regarding application of metagenomics to study complex bacterial populations and to compare populations by metabarcoding.
- Ability to select the most appropriate tools for statistical processing, visualization and comparison of metagenomic datasets. The students will know how to assure a statistical reliability of research conclusions derived from a metagenomics project and at which Web-based databases the obtained metagenomic datasets should be deposited prior to publication.

BACKGROUND KNOWLEDGE REQUIRED

Basic knowledge of microbiology and genetics; computer literacy.

TEACHING METHODS/APPROACH

The course will be taught using lectures and practical exercises.

BOOKS & OTHER SOURCES USED

No textbooks are needed for this course. Lectures were prepared based on recent reviews and publications in open-source peer-reviewed journals.

COURSE CONTENT

5. Introduction to metagenomics;
6. Consideration of several famous metagenomics projects and Web-portals;
7. Amplicon based and whole genome sequencing metagenomics;
8. Species diversity identification vs. functional metagenomics;
9. Read binning approaches, the lowest common ancestor concept;
10. Sequenced based and composition based binning; unsupervised and supervised binning;

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11. Metagenomics software tools: MEGAN, Sort-ITEM, SOM, GOHTAM and others.
12. Processing of reads generated by NGS for metagenomics and metabarcoding;
13. Rarefaction analysis, identification and removal of chimeric sequences and dereplication; other statistical procedures and visualization approaches;
14. Web resources for deposition of metagenomic dataset and for comparative studies: Camera, MG-RAST, Human Microbiome Project, MEGAN-DB

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

1. Practical test: 25%
2. Written assignment: 75%

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