

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

MSc PROGRAMME OUTLINE

MSc in Bioinformatics and Computational Molecular Biology

Course Work / Project Masters	Year: 2015	Coordinator: Prof Özlem TAŞTAN BISHOP
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COURSE WORK and RESEARCH THESIS MASTERS

in

**BIOINFORMATICS and
COMPUTATIONAL MOLECULAR BIOLOGY**

2015

DEPARTMENTS

of

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

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ORIENTATION DAY

(12 February 2015, Thursday)

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

09:00 – 9:30	Welcoming and introduction of students, lecturers, supervisors, rest of RUBi members
09:30 – 10:00	“Introduction to the programme” by Prof Özlem Taştan Bishop
10:00 – 10:30	“What is plagiarism?” by Prof Philip Machanick <i>(Please see pages 18 and 19 in this document)</i>
10:30 – 11:00	Tea break
11:00 – 12:00	Research talks with some examples from previous MSc projects <ul style="list-style-type: none">• 11:00 - Kevin Lobb• 11:20 - Philip Machanick• 11:40 - Prof Özlem Taştan Bishop
15:00 – 17:00	Laptops will be given to the students who completed the registration process (RUBi Lab 129A)

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PROPOSED PROGRAMME FOR 2015

Date	Module	Content
12 Feb, Thu	ORIENTATION DAY	
13 Feb, Fri	Research project discussion with supervisor(s) <i>(Time will be arranged by supervisors)</i>	
16 Feb, Mon - 20 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
23 Feb, Mon – 27 Feb, Fri [25 hours]	Basic Genomics Prof Özlem Taştan Bishop	DNA and protein databases; database searching; sequence alignment
2 Mar, Mon – 6 Mar, Fri [10 hours]	Introduction to Programming Prof Denis Pollney	Basics for (Python) programming
9 Mar, Mon – 10 Mar, Tue [10 hours]	Introduction to Mathematics Prof Özlem Taştan Bishop	Review of basic calculus and linear algebra

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11 Mar , Wed – 13 Mar , Fri [15 hours]	Mathematical Programming Prof Nigel Bishop	The MATLAB computational environment, MATLAB scripts, graphical output, functions, systems of linear and non-linear equations, differential equations. Use of the Bioinformatics Toolbox.
16 Mar , Mon – 2 Apr , Thu [75 hours]	Python for Bioinformatics Mr Gustavo Adolfo Salazar Orejuela	<ul style="list-style-type: none"> • Introductory and advanced Python • Biopython
3 Apr , Fri – 6 Apr , Mon	Easter holiday	
7 Apr , Tue – 11 Apr , Friday	Python (assignment week)	
13 Apr , Mon – 17 Apr , Fri [25 hours]	Databases Mr Rowan Hatherley Mr David Brown	<ul style="list-style-type: none"> • Introduction to databases • Introduction to web frameworks • MySQL; Django
20 Apr , Mon - 25 Apr , Fri	Study week	

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28 Apr, Tue – 9 May, Fri	EXAMINATIONS: <ul style="list-style-type: none"> • Linux (28 April) • Basic genomics (29 April) • Basic mathematics and mathematical programming (30 April) • Python (1 May) • Databases (2 May) 	
4 May, Mon - 8 May, Fri [25 hours]	Structural Bioinformatics I Dr Kevin Lobb	Molecular dynamics; protein-small molecule interactions; Autodock.
11 May, Mon - 15 May, Fri [25 hours]	Statistics Mr Jeremy Baxter	Introductory statistics; R: statistical software
18 May, Mon - 22 May, Fri [25 hours]	Metagenomics Prof Oleg Reva	<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;
25 May, Mon - 29 May, Fri	Study week	
1 June, Mon– 5 June, Fri [25 hours]	Structural Bioinformatics II Prof Özlem Taştan Bishop	Structural bioinformatics techniques; homology modeling
8 June, Mon – 12 June, Fri [25 hours]	Genome Wide Association Studies Dr Emilson Chimusa	Introduction to diseases scoring statistics, medical population structure and advanced data analysis

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15 June, Mon – 19 June, Fri	Study week
22 Jun, Mon – 26 Jun, Fri	EXAMINATIONS: <ul style="list-style-type: none"> • Structural Bioinformatics I (22 June) • Structural Bioinformatics II (23 June) • Statistics (24 June) • Metagenomics (25 June) • GWAS (26 June)
29 Jun, Mon – 12 Jul, Sun	BREAK
15 Jul, Wed	PROJECTS: Hand-in Literature Review and Project Proposal to Supervisor and Co-supervisor – Project starts!
Week of 20 Jul	PROJECTS: Project Proposal Presentations
29 Jul, Wed – 18 Nov, Wed	BIOINFORMATICS JOURNAL CLUB
Week of 21 Sep	1 st Presentation of Project Progress
Week of 19 Oct	2 nd Presentation of Project Progress
Week of 31 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	20	8	12
Introduction to Mathematics	10	7	3
Mathematical programming	15	5	10
Basic Genomics	25	12	13
Python for Bioinformatics	75	30	45
Databases	25	10	15
Structural Bioinformatics I	25	11	14
Structural Bioinformatics II	25	11	14
Metagenomics	25	11	14
Statistics	25	10	15
GWAS	25	11	14
TOTAL	295	116	179

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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)
Introduction to Linux	6.7 %	2
Basic and Advanced Genomics I	8.5%	3
Mathematics & Mathematical programming	8.5%	3
Python for Bioinformatics	25.3%	4-5
Databases	8.5%	3
Structural Bioinformatics I	8.5%	3
Structural Bioinformatics II	8.5%	3
Metagenomics	8.5%	3
Statistics	8.5%	3
GWAS	8.5%	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:

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: 40%
2. Test 2: 60%

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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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INTRODUCTION TO PROGRAMMING

Lecturer: Prof Denis Polney

Contact hours: 10

This is an introductory module to prepare students for programming. Students will not be examined on this module.

SPECIFIC OUTCOMES ADDRESSED

1. Learn the basic syntax of the Python programming languages
2. Be able to use Python variables, loops, and logical operations
3. Write short programs to accomplish some simple calculations and tasks

BACKGROUND KNOWLEDGE REQUIRED

1. How to use the Linux command line and directory structure
2. Editing files in Linux

TEACHING METHODS/APPROACH

We begin each lecture with a short introductory discussion introducing new concepts. We then work through a set of practical problem sets which make use of the concepts. Please bring laptops to the lectures.

BOOKS & OTHER SOURCES USED

None required. Available online resources will be indicated during the lectures.

COURSE CONTENT

1. Python variables: integers, floating point numbers and strings
2. Simple string manipulation
3. Logical operations on variables
4. Loops and control structures
5. Input/output methods

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BASIC MATHEMATICS

Lecturer: Prof Özlem Taştan Bishop

Contact hours: 10

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. Assignment: 50%
2. Test: 50%

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MATHEMATICAL PROGRAMMING WITH MATLAB

Lecturer: Prof Nigel T. Bishop

Contact hours: 15

SPECIFIC OUTCOMES ADDRESSED

1. Introduction to mathematical programming with MATLAB.
2. Solve problems using mathematical programming.

BACKGROUND KNOWLEDGE REQUIRED

Matrix algebra, basic calculus.

TEACHING METHODS/APPROACH

Lectures will be mainly in the form of demonstrations of MATLAB features, with discussion. Relevant notions from various aspects of mathematics will be discussed as necessary. At each lecture a set of exercises will be presented, which students should complete and submit by the next lecture.

BOOKS & OTHER SOURCES USED

Course notes.

Essential MATLAB for Scientists and Engineers, B Hahn, Pearson, 3rd edition ISBN 1 868 91143 82

COURSE CONTENT

The purpose of the course is to enable the student to construct a computational environment with MATLAB in which to model, study and simulate real-world processes. It is intended that the student learn this skill by hands-on experience with the computer. The lectures are meant to provide an overview and a forum for discussion. The exercises are there to provide practical experience. Most of the real learning will be accomplished by doing the exercises.

1. Introduction to the MATLAB environment; programming in MATLAB: statements, data structures, input / output, flow control, functions, graphics.
2. Linear algebra with MATLAB: systems of equations, over-determined systems and linear regression, eigenvalues and eigenvectors. Other applications: differentiation, integration, solving nonlinear equations and differential equations.
3. Introduction to MATLAB's Bioinformatics Toolbox.

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

1. Assignment 1: 20%
2. Assignment 2: 20%
3. Project: 60%

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PYTHON AND BIOPYTHON

Lecturer: Mr Gustavo Salazar

Contact hours: 75

SPECIFIC OUTCOMES ADDRESSED

1. To be able to write short Python program to manipulate data
2. To understand the differences between numbers, strings, lists and arrays
3. To master the use of various control structures and functions within Python program
4. To understand the concepts of the Object Oriented paradigm and how to use it in python
5. To retrieve and manipulate data from databases and files
6. To use the most common procedures in Biopython

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

Lectures: utilizing self-study tutorials and demonstration programmes
Numerous small exercises to build up experience and skills progressively

BOOKS & OTHER SOURCES USED

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

Biopython <http://biopython.org/wiki/Biopython>

COURSE CONTENT

1. Introduction to Python (Thinking, writing and running)
2. Flow Control
3. Data Structures
4. Strings in Depth
5. Functions
6. Importing Standard Modules
7. Files for Input and Output
8. Regular Expressions
9. Basic Parsing
10. Exceptions and error handling
11. Recursion
12. Classes and Objects
13. Database Theory and Relational Databases
14. Biopython
15. Graphical User Interfaces

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ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

1. Test: 30%
 2. Mini-project: 30%
- Assignments: 40%

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DATABASES

Lecturers: Mr David Brown and Mr Rowan Hatherley

Contact hours: 25

SPECIFIC OUTCOMES ADDRESSED

1. To understand what databases are and why they are used
2. To be able to create and manage a simple database using MySQL
3. To understand what a web framework is and why it is used
4. To create simple web pages using Django
5. To create and manage a simple online database using Django and MySQL

BACKGROUND KNOWLEDGE REQUIRED

1. Basic computer literacy
2. Basic Python programming skills

TEACHING METHODS/APPROACH

Teaching will consist of lectures, practicals and tutorials.

BOOKS & OTHER SOURCES USED

Course notes and lecture slides, The Django website (www.djangoproject.com), the MySQL website (www.mysql.com), <http://www.w3schools.com>, other web searches and online tutorials

COURSE CONTENT

1. Introduction to databases and DBMs
2. Database design
3. SQL and MySQL
4. Introduction to web frameworks
5. Django

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

- | | |
|-----------------------------------|-----|
| 1. Daily practicals and tutorials | 60% |
| 2. Test | 20% |
| 3. Assignment | 20% |

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STRUCTURAL BIOINFORMATICS – I

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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STRUCTURAL BIOINFORMATICS – II

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 Baxevanis 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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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

1. Introduction to metagenomics;
2. Consideration of several famous metagenomics projects and Web-portals;
3. Amplicon based and whole genome sequencing metagenomics;
4. Species diversity identification vs. functional metagenomics;
5. Read binning approaches, the lowest common ancestor concept;

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6. Sequenced based and composition based binning; unsupervised and supervised binning;
7. Metagenomics software tools: MEGAN, Sort-ITEM, SOM, GOHTAM and others.
8. Processing of reads generated by NGS for metagenomics and metabarcoding;
9. Rarefaction analysis, identification and removal of chimeric sequences and dereplication; other statistical procedures and visualization approaches;
10. 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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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

11. Basic Calculus: Differentiation and integration
12. Linear algebra: Matrices, vectors
13. Matlab literacy, specifically matrix operations.
14. 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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GENOME WIDE ASSOCIATION STUDIES (GWAS)

Lecturer: Dr Emilson Chimusa (<http://www.cbio.uct.ac.za/emile-chimusa/>)

Contact hours: 25

SPECIFIC OUTCOMES ADDRESSED

This course is devoted to computational problems and methods in the emerging field of Medical population genetics and disease scoring statistics (Genome-wide Associations Studies) where genomics, computational biology and both Biostatistics and Bioinformatics impact medical research. In addition, this course will also provide a forum for statistical and biological students to exchange their ideas, problems, and thoughts in a free, stimulating atmosphere. The students in this course will receive the most rigorous training at the interplay between disease scoring statistics and medical genetic discoveries. Students will be able to solve genetic mysteries with the obtained quantitative skills and gain insight in new developments in the field of genome wide association studies. Students will be empowered with knowledge on statistical and computational details to facilitate genetic data analyses and result interpretations.

BACKGROUND KNOWLEDGE REQUIRED

The module is designed for graduate students with some background in Calculus. Understanding of basic in the genetic epidemiology and Statistics include

1. Regression analysis, mixed model.
2. Maximum likelihood estimation.
3. Bayesian statistics (desirable).
4. programming Skill in python, R.
5. Familiarity with basic genetics is desirable.

Experience in working with the Linux command line interface.

TEACHING METHODS/APPROACH

Since the course will be comprised of students with a diverse background, homework and tests will involve general questions for all students as well as more in-depth questions, which students will be able to choose from in accordance with their particular background. Mainly the lectures will be split equally between lectures and tutorials, self study, article discussions and student presentations.

BOOKS & OTHER SOURCES USED

A. Books

Principles of Population Genetics (Fourth Edition, 2007) Daniel L. Hartl and Andrew G. Clark.

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Statistical Genetics of Quantitative Traits: Linkage, Maps, and QTL by Rongling Wu Chang-Xing Ma, and George Casella. Springer-Verlag, New York (2007).

B. Articles

Chimusa ER, Daya M, Moller M, Ramesar R, Henn BM, et al. (2013) Determining Ancestry Proportions in Complex Admixture Scenarios in South Africa Using a Novel Proxy Ancestry Selection Method. PLoS ONE 8(9): e73971. doi:10.1371/journal.pone.0073971.

Chimusa ER, Noah Zaitlen, Michelle Daya, Marlo Moller, Paul D. van Helden, Nicola J. Mulder, Alkes L. Price, and Eileen G. Hoal. "Genome-wide association study of ancestry-specific TB risk in the South African Coloured population." Human molecular genetics 23, no. 3 (2014): 796-809.

Albers CA, Lunter G, MacArthur DG, McVean G, Ouwehand WH, Durbin R (2010) Dindel: accurate indel calls from short-read data. Genome Res. 21:961-73.

Browning SR, Browning BL (2007) Rapid and accurate haplotype phasing and missing-data inference for whole-genome association studies by use of localized haplotype clustering. Am J Hum Genet. 81:1084-97. PMID: 17924348.

Coventry A, Bull-Otterson LM, Liu X, Clark AG, Maxwell TJ, Crosby J, Hixson JE, Rea TJ, Muzny DM, Lewis LR, Wheeler DA, Sabo A, Lusk C, Weiss KG, Akbar H, Cree A, Hawes AC, Newsham I, Varghese RT, Villasana D, Gross S, Joshi V, Santibanez J, Morgan M, Chang K, Iv WH, Templeton AR, Boerwinkle E, Gibbs R, Sing CF (2010) Deep resequencing reveals excess rare recent variants consistent with explosive population growth. Nat Commun. 1:131. PMID: 21119644.

Delaneau O, Zagury JF, Marchini J (2013) Improved whole-chromosome phasing for disease and population genetic studies. Nat Methods. 10:5-6. PMID: 23269371.

Howie B, Fuchsberger C, Stephens M, Marchini J, Abecasis GR (2012) Fast and accurate genotype imputation in genome-wide association studies through pre-phasing. Nat Genet. 44:955-9. PMID: 22820512.

Iqbal Z, Caccamo M, Turner I, Flicek P, McVean G (2012) De novo assembly and genotyping of variants using colored de Bruijn graphs. Nat Genet. 44:226-32. PMID: 22231483.

Jun G, Flickinger M, Hetrick KN, Romm JM, Doheny KF, Abecasis GR, Boehnke M, Kang HM (2012) Detecting and estimating contamination of human DNA samples in sequencing and array-based genotype data. Am J Hum Genet. 91:839-48. PMID: 23103226.

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Li H, Ruan J, Durbin R (2008) Mapping short DNA sequencing reads and calling variants using mapping quality scores. *Genome Res.* 18:1851-8. PMID: 18714091.

Li H, Durbin R (2009) Fast and accurate short read alignment with Burrows-Wheeler transform. *Bioinformatics.* 25:1754-60. PMID: 19451168.

Li H, Durbin R (2011) Inference of human population history from individual whole-genome sequences. *Nature.* 475:493-6. PMID: 21753753.

Li Y, Willer CJ, Ding J, Scheet P, Abecasis GR (2010) MaCH: using sequence and genotype data to estimate haplotypes and unobserved genotypes. *Genet Epidemiol.* 34:816-34. PMID: 21058334.

Lin DY, Zeng D (2010) Meta-analysis of genome-wide association studies: no efficiency gain in using individual participant data. *Genet Epidemiol.* 34:60-6. PMID: 19847795.

Liu et al (2013) <http://arxiv.org/abs/1305.1318>.

Wen X, Stephens M (2010) Using linear predictors to impute allele frequencies from summary or pooled genotype data. *Ann Appl Stat.* 4:1158-1182. PMID: 21479081.

Wu MC, Lee S, Cai T, Li Y, Boehnke M, Lin X (2011) Rare-variant association testing for sequencing data with the sequence kernel association test. *Am J Hum Genet.* 89:82-93.

Zerbino DR, Birney E (2008) Velvet: algorithms for de novo short read assembly using de Bruijn graphs. *Genome Res.* 18:821-9. PMID: 18349386.

COURSE CONTENT

Medical Population Genetic
Imputation
Statistical analysis of quantitative genetics
Genome-wide association studies
Local ancestry inference and Admixture Mapping

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

1. Projects: 50%
2. Homeworks: 35%
3. Presentation: 15%

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