

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

MSc PROGRAMME OUTLINE

MSc in Bioinformatics and Computational Molecular Biology

Course / Project Work Masters	Year: 2011	Coordinator: Dr Özlem TAŞTAN BISHOP
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COURSE WORK and RESEARCH PROJECT MASTERS

**BIOINFORMATICS and
COMPUTATIONAL MOLECULAR BIOLOGY**

2011

DEPARTMENTS

of

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

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ORIENTATION PROGRAMME

DATE	PROGRAMME
7 Feb, Mon	10h30-11h00: Welcome and short meeting at RUBi 11h00-12h00: Brief campus tour (Locations of Library, Student office etc.) 12h00-1230: Meet Prof George Wells (HOD, Computer Science) at the Department of Computer Science 12h30-13h00: Meet Prof. Nigel Bishop (HOD, Mathematics) at the Department of Mathematics 14h30-15h00: Meet Dr. Kevin Lobb at the Department of Chemistry 15h00-15h30: Meet Mr. Jeremy Baxter at the Department of Statistics
8 Feb, Tue	08h30-10h30: Research methodology (Prof Peter Rose, EBRU) * 10h30-11h00: Tea break 14h00-15h00: Introduction to data & statistics analysis (Mr Jeremy Baxter, Department of Statistics) * 16h00-17h00: Departmental meeting 2011 (Entire Department) ** After DM : Welcoming braai and drinks (Entire Department)
9 Feb, Wed	09h00-10h15: Library information literacy workshop (Ms Eileen Sheperd, Principal Librarian, Rhodes University) 11h00-13h00: Research methodology-part 2 (Prof Peter Rose, EBRU) * 14h00-15h00: Introduction to data presentation and scientific writing (Open Discussion – Prof Janice Limson, Dr Earl Prinsloo) *
10 Feb, Thu	Free
11 Feb, Fri	9h00-10h00: Tutor workshop (Tea Room) 11h00-11h30: Outline of the overall MSc programme 11h30-12h00: Selecting office/working space at RUBi, handing computers 12h00-12h30: Introduction to management of computational data (Dr. O. Tasthan Bishop)

* Tea Room, ** Zoo Minor 1 Lecture Theatre

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PROPOSED PROGRAMME FOR 2011

Date	Module	Content
7 Feb, Mon - 11 Feb, Fri	ORIENTATION WEEK	
14 Feb, Mon - 17 Feb, Thu [20 hours]	Introduction to Linux Dr. Özlem Taştan Bishop	<ul style="list-style-type: none"> • Use of Linux and Linux shell commands • Operating systems (e.g. OpenSUSE, Fedora) • Software installation <p>* Students will install the Linux operating system to their laptop and required programs</p>
18 Feb, Fri	University orientation programme	
21 Feb, Mon – 25 Feb, Fri [20 hours]	Basic Genomics Dr Özlem Taştan Bishop	DNA and protein databases; Database searching using text and sequence based search formats; Sequence alignment; Domain and motif searches; Gene and promoter prediction
25 Feb, Fri [2 hours]	Project Discussion Dr Özlem Taştan Bishop	Project discussion on project proposal preparation
25 Feb, Fri – 13 Jun, Mon	PROJECTS: Selection of project; Literature review; Project proposal preparation and presentation	
28 Feb, Mon - 4 Mar, Fri [25 hours]	Structure & Function of Biomacromolecules – Part 1 Dr Özlem Taştan Bishop	Structural biology techniques; Template and non-template based protein structure prediction methods; Homology modeling; Modeler; Protein-protein interactions; Protein visualization programs

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7 Mar, Mon – 11 Mar, Fri	Self study	
14 Mar, Mon – 18 Mar, Fri [10 hours]	Structure & Function of Biomacromolecules – Part 2 Dr Adrienne Edkins	Rational and a-rational protein/enzyme engineering; Oligonucleotide-based mutagenesis.
21 Mar, Mon – 25 Mar, Fri	Self study	
28 Mar, Mon - 1 Apr, Fri [10 hours]	Phylogenetics Dr Michael Ludewig	Introduction to phylogenetics; Programs for phylogenetics; Applications
4 Apr, Mon – 8 Apr, Fri	Self study	
11 Apr, Mon – 15 Apr, Fri [25 hours]	Structure & Function of Biomacromolecules – Part 3 Dr Kevin Lobb	NMR; Molecular dynamics; Protein-small molecule interactions; Autodock.
18 Apr, Mon - 21 Apr, Thu [16 hours]	Introduction to Mathematics with Biological Applications Dr Özlem Taştan Bishop	Basic Calculus: Differentiation, integration Linear algebra: Matrices, eigenvalue – eigenvector problems Introduction to differential equations: Chemical reactions, population models
22 Apr, Fri – 25 Apr, Mon	Easter Break	
26 Apr, Tue – 29 Apr, Fri [20 hours]	Mathematical Programming Prof. Nigel Bishop	The MATLAB computational environment, MATLAB scripts, matrix operators, graphical output, functions, systems of linear equations, eigenvalues, differential equations, bioinformatics toolkit

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2 May , Mon - 13 May Fri [40 hours]	Python for Bioinformatics Mr. Gustavo Adolfo Salazar Orejuela	Introductory and advance Python; Biopython
16 May , Mon - 17 May Tue [12 hours]	Databases Prof. Fourie Joubert	Mass storage of data, classic file handling techniques, modern databases and MySQL and Turbogears commands.
18 May , Wed - 20 May Fri [18 hours]	Advance Genomics Prof. Fourie Joubert	Genome annotation, Genome assembly and analysis, Comparative Genomic
23 May , Mon – 27 May , Fri	Self study	
30 May , Mon - 3 June Fri [20 hours]	Statistics – Part 1 Mr. Jeremy Baxter	Introductory statistics; R: Statistical Software
6 Jun , Mon – 8 Jun , Wed [12 hours]	Statistics – Part 2 Prof. Gunther Jäger	Hidden Markov Models (HMMs)
10 Jun , Fri	PROJECTS: Hand-in Literature Review and Project Proposal to Supervisor and Co-supervisor	
13 Jun , Mon	PROJECTS: Project Proposal Presentations	
20 Jun , Mon – 28 Jun , Tue	EXAMINATIONS	
1 Jul , Fri	Exam Results	
11 Jul , Mon	PROJECTS: Start	

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1 Aug , Mon – 18 Nov , Fri	BIOINFORMATICS JOURNAL CLUB (Every week, one research paper will be presented by a student – open to all Science Departments)
29 Aug , Mon – 2 Sep , Fri	PROJECTS: Presentation of Project Progress
28 Nov , Mon – 2 Dec , Fri	PROJECTS: Presentation of Project Results
12 Dec , Mon	PROJECTS: Hand-in Thesis

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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 12 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 overall course-work and the research work will each contribute 50% to an overall mark.

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
Introduction to Linux	8.1%	1 hour 30 mins
Basic Genomics	8.1%	1 hour 30 mins
Structure and Function of Biomacromolecules – Part 1	10.1%	1 hour 30 mins
Structure and Function of Biomacromolecules – Part 2	4.0%	1 hour
Phylogenetics	4.0%	1 hour
Structure and Function of Biomacromolecules – Part 3	10.1%	1 hour 30 mins
Introduction to Mathematics-Biological Applications	6.5%	1 hour 30 mins
Python for Bioinformatics	16.1%	2 hours 30 mins
Databases	4.8%	1 hour
Advance Genomics	7.2%	1 hour 30 mins
Mathematical Programming	8.1%	1 hour 30 mins
Statistics – Part 1	8.1%	1 hour 30 mins
Statistics – Part 2	4.8%	1 hour

A student whose overall coursework mark is less than 50% will be deemed to have failed the programme. In addition, a student getting less than 40% in two or more modules, at the discretion of the Department, may also be deemed to have failed the programme.

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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 presentation 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: 10-15 typed pages. Include sections on: Literature review (5–10 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
Acknowledgments
Introduction
Methods
Results and Discussion
Conclusion
References

Dates

As specified in the programme earlier in this manual.

ASSESSMENT CRITERIA & PROCEDURE

The thesis will be assessed by two external examiners.

NUMBER OF COPIES OF THE RESEARCH REPORT

You should prepare three copies of your thesis.

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

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of the investigation; (ii) state the methodology used; (iii) summarize the results; (iv) state the principal conclusions. It should not exceed 250 words as a single paragraph.

2. INTRODUCTION

Literature review

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

Project hypothesis, aims & objectives and motivation

A clear statement of the hypothesis and aims & objectives of the project and motivation for these.

3. METHODOLOGY

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

4. RESULTS AND DISCUSSION

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. REFERENCE

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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MSc Proposal Presentation Evaluation Form

Criterion	Weight	Mark
Concise, accurate & up-to-date literature review	20	
Knowledge gap and/or problem clearly identified and stated	20	
Clear research hypothesis & objectives; Concise description of approach and methods	20	
Research objectives, approach & methods. Realistic? Feasible?	15	
Time management, visual media and speaker – audience contact	10	
Ability of speaker to answer questions in a clear & meaningful manner.	15	
Total	100	

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MSc Written Proposal Evaluation Form

Criterion	Weight	Mark
Concise, accurate & up-to-date literature review	30	
Knowledge gap and/or problem clearly identified and stated	20	
Clear research hypothesis & objectives; Concise description of approach and methods	20	
Research objectives, approach & methods. Realistic? Feasible?	15	
Quality of scientific writing	15	
Total	100	

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MSc Project Presentation Evaluation Form

Criterion	Weight	Mark
Concise, accurate & up-to-date literature review	15	
Knowledge gap and/or problem clearly identified and stated	15	
Clear research hypothesis & objectives; Concise description of approach and methods	15	
Results and discussion: interpretation of results and critical analysis of their meaning and impact	25	
Summary of findings and future plans	5	
Time management, visual media and speaker – audience contact	10	
Ability of speaker to answer questions in a clear & meaningful manner.	15	
Total	100	

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COURSE WORK MODULES

INTRODUCTION TO LINUX

Lecturer: Dr Özlem Taştan Bishop

Dates: 14 February to 18 February 2011

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 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

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ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

1. Test 1: 40%
2. Test 2: 60%

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BASIC GENOMICS

Lecturer: Dr Özlem Taştan Bishop

Dates: 21 February to 25 February 2011

Contact hours: 20

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
4. Learn about prediction algorithms, programs and apply it in gene and protein level

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

COURSE CONTENT

1. Introduction to bioinformatics
2. Biological databases
3. Sequence alignment
 - a. Pairwise sequence alignment
 - b. Database similarity search
 - c. Multiple sequence alignment
 - d. Profiles and HMMs
 - e. Protein motifs and domain predictions
4. Gene prediction
5. Promoter and regulatory element prediction

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

1. Assignment 1: 20%
2. Assignment 2: 20%
3. Assignment 3: 20%
4. Test: 40%

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STRUCTURE AND FUNCTION OF BIOMACROMOLECULES: PART 1

Lecturer: Dr Özlem Taştan Bishop

Dates: 28 February to 4 March 2011

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 about protein-protein docking methods

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
6. Protein-protein docking

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

1. Assignment 1: 20%
2. Assignment 2: 20%
3. Assignment 3: 20%
4. Test: 40%

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STRUCTURE AND FUNCTION OF BIOMACROMOLECULES: PART 2

Lecturer: Dr Adrienne Edkins

Dates: 14 March to 18 March 2011

Contact hours: 10

SPECIFIC OUTCOMES ADDRESSED

After completing this course, the student should be able to:

1. Understand the link between protein structure and function
2. Use bioinformatics to evaluate the link between structure and function
3. Critically evaluate scientific literature
4. Communicate scientific data effectively

BACKGROUND KNOWLEDGE REQUIRED

1. Ability to draw and describe the key biochemical properties of the side chains of all amino acids, especially the key functional groups and their different ionization states.
2. Basic understanding of the primary, secondary, tertiary and quaternary structure of proteins, and the various non-covalent bonds involved in the formation of secondary, tertiary and quaternary structures.
3. Basic understanding of the structure of different forms of nucleic acids, including the biochemical modification of nucleic acids.
4. Ability to identify the key genetic elements of a gene and the processes involved in gene expression, especially the coding region, transcriptional elements & transcription, and translational elements & translation.
5. An understanding of:
 - a. Restriction endonucleases and how they work;
 - b. Agarose gel electrophoresis and how this technique is used to separate DNA fragments;
 - c. The polymerase chain reaction and;
 - d. The DNA sequencing reaction, what its components are and how it works.

TEACHING METHODS/APPROACH

Formal lectures will be complemented by self-study, active learning assignments and participative journal clubs in which students will be expected to work independently and contribute to group discussions and presentations.

BOOKS & OTHER SOURCES USED

There is no formal textbook for this course.

Limited lecture notes and background reading/journal articles will be provided which

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students should supplement with additional reading from additional journals and library resources as necessary.

COURSE CONTENT

1. Rational and arational protein engineering
2. Protein engineering strategies
3. Site directed mutagenesis

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

This course will be assessed by assignments as indicated below.

ASSESSMENT MECHANISM	PROPORTION OF FINAL MARK
Protein engineering exercise [written and presentation]	30%
Oligonucleotide design exercise [written and presentation]	30%
Written Journal club tutorial	30%
Overall attitude and contribution to class	10%
TOTAL	100%

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PHYLOGENETIC ANALYSIS

Lecturer: Dr Michael Ludewig

Dates: 28 March to 1 April 2011

Contact hours: 10

SPECIFIC OUTCOMES ADDRESSED

1. Introduction to the concepts of molecular phylogenetics
2. Understand phylogenetic trees
3. Generation and interpretation of phylogenetic trees using computer programmes
4. Development of an understanding of the potential applications of phylogenetics

BACKGROUND KNOWLEDGE REQUIRED

1. Generation of multiple sequence alignment
2. Familiarity with genome databases, protein and DNA sequence data

TEACHING METHODS/APPROACH

There will be a component of self study and practical assignments involving the generation and interpretation of phylogenetic data.

BOOKS & OTHER SOURCES USED

1. Bioinformatics and Molecular Evolution, Higgs, P.G. and Attwood, T.K., Blackwell Publishing.
2. Understanding Bioinformatics, Zvelebil, M. and Baum, J.O. Garland Science, Taylor & Francis Group.
3. The Phylogenetic Handbook: A Practical Approach to DNA and Protein Phylogeny, Edited by Salemi, M. and Vandamme, A-M. Cambridge University Press.
4. Phylogenetics: the Theory and Practice of Phylogenetic Systematics. E.O. Wiley, John Wiley and Sons.

COURSE CONTENT

This course is designed to introduce students to phylogenetics and associated computer software.

1. Introduction to phylogenetics concepts
2. Methods of phylogenetic inference
3. The applications of phylogenetics data
4. Practical usage of phylogenetics programmes

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

This course will be assessed by assignments.

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STRUCTURE AND FUNCTION OF BIOMACROMOLECULES: PART 3

Lecturer: Dr. Kevin A. Lobb

Dates: 11 April to 15 April 2011

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.

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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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INTRODUCTION TO MATHEMATICS WITH BIOLOGICAL APPLICATIONS

Lecturer: Dr Özlem Taştan Bishop

Dates: 18 April to 21 April 2011

Contact hours: 16

SPECIFIC OUTCOMES ADDRESSED

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

BACKGROUND KNOWLEDGE REQUIRED

Basic mathematics

TEACHING METHODS/APPROACH

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

BOOKS & OTHER SOURCES USED

Lecture notes

Any Calculus, Linear Algebra and Differential Equation books

COURSE CONTENT

1. Calculus (Differentiation and integration)
2. Linear Algebra (Matrices, eigenvalue / eigenvector problems)
3. Introduction to differential equations

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

1. Assignment 1: 20%
2. Assignment 2: 15%
3. Assignment 3: 15%
4. Test: 50%

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MATHEMATICAL PROGRAMMING WITH MATLAB

Lecturer: Prof Nigel T Bishop

Dates: 26 April to 29 April 2011

Contact hours: 20

SPECIFIC OUTCOMES ADDRESSED

1. Introduction to mathematical programming with MATLAB.
2. Solve real-world problems using mathematical programming.
3. Knowledge of the MATLAB computational environment. In particular, to: write scripts; perform linear and non-linear regression; deal with iterative processes.
4. Introduction to the MATLAB Bioinformatics toolbox

BACKGROUND KNOWLEDGE REQUIRED

Computer programming in any other language.

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

Essential MATLAB for Scientists and Engineers, B Hahn, Pearson, 3 rd 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. Some of the exercises are designed to get the student to extend theory or develop new techniques on his / her own. Most of the real learning will be accomplished by doing the exercises.

1. Introduction to the MATLAB environment
2. Matrix algebra, functions in MATLAB
3. Generating lists, matrices, random matrices, addressing parts, products and sums, augmenting, reshaping, higher-dimensional arrays
4. MATLAB scripts, matrix operators, logical matrices
5. Graphical output
6. Flow control, while loops, switch-case, functions
7. Systems of linear equations, linear and general regression and data analysis with MATLAB

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8. Numerical analysis: solution of nonlinear equations, numerical differentiation and integration, polynomials, interpolation
9. The Bioinformatics toolbox

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

1. Assignment 1: 20%
2. Assignment 2: 20%
3. Assignment 3: 20%
4. Assignment 4: 40%

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PYTHON AND BIOPYTHON

Lecturer: Gustavo Salazar

Dates: 2 May to 13 May 2011

Contact hours: 40

SPECIFIC OUTCOMES ADDRESSED

1. To be able to write short Python Programmes 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 Programmes
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

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15. Graphical User Interfaces

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

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

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DATABASES

Lecturer: Prof Fourie Joubert

Dates: 16 May to 17 May 2011

Contact hours: 12

SPECIFIC OUTCOMES ADDRESSED

1. Understanding the need for relational databases
2. Understanding the structure of relational databases
3. Understanding Structured Query Language

BACKGROUND KNOWLEDGE REQUIRED

1. Basic computer knowledge
2. Python programming knowledge.

TEACHING METHODS/APPROACH

1. The course will be taught over two days from 8:30 to 16:30
2. It will include theory and practical sessions.

BOOKS & OTHER SOURCES USED

1. Database Systems by Connolly & Begg
2. Free Internet sources

COURSE CONTENT

The course is aimed at introducing students to relational databases. It will explain the need for structured databases systems, together with their advantages and disadvantages. It will then explore relational databases together with the necessary language aspects for use of these systems.

1. Introduction to databases
2. Databases and database management systems
3. Database design
4. Database relations
5. Structured Query Language

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

Completion of assignment: 100%

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ADVANCED GENOMICS

Lecturer: Prof Fourie Joubert

Dates: 18 May to 20 May 2011

Contact hours: 18

To be advised

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INTRODUCTORY STATISTICS

Lecturer: Mr. Jeremy Baxter

Dates: 30 May to 3 June 2011

Contact hours: 20

Lecturer: Prof. Gunther Jäger

Dates: 6 June to 8 June 2011

Contact hours: 12

SPECIFIC OUTCOMES ADDRESSED

The aims of this course are:

1. To provide students with an introduction to statistics in order to solve problems of bioinformatics.
2. 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.
3. To provide students with the theory and application of Hidden Markov Models.

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.
9. Understand and apply the theory of Hidden Markov Models.

BACKGROUND KNOWLEDGE REQUIRED

1. Basic Calculus: Differentiation and integration
2. Linear algebra: Matrices, eigenvalues and eigenvectors

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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.

BOOKS & OTHER SOURCES USED

1. J Baxter, Introductory Statistics for Bioinformaticians using R (course notes/slides).
2. G Jäger, Markov chains and Hidden Markov models (course notes).
3. 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)
6. Markov chains: basic properties, concepts and examples.
7. Hidden Markov models: backward and forward algorithm, Viterbi algorithm, Baum-Welch algorithm, applications.

ASSESSMENT ACTIVITIES AND THEIR WEIGHTS

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

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