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## Advanced Diploma Programme in Modeling and Simulation

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## About This Document

This document outlines an academic programme, the Advanced Diploma Programme in Modeling and Simulation, designed by the people at the Centre for Modeling and Simulation, University of Pune, and approved by the University of Pune.

## Citing This Document

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#### Abstract

About the Centre The Centre for Modeling and Simulation, University of Pune, was established in August 2003 to promote, support and facilitate academic and research activities that use modeling, simulation and computation as the "third scientific methodology" (besides theory and experiment) and transcend the traditional boundaries separating established scientific disciplines. At the time of writing this document, the Centre possesses three full-time faculty, one postdoctoral fellow, a small support staff, plus considerable computational expertise and resources. For more information about the Centre, please visit our website http://cms.unipune.ernet.in/.


## Acknowledgments

Many people have contributed to the creation of this document and this programme. Their time and effort, contributions and insights, and comments and suggestions have all gone a long way towards bringing this document to its present form. The Centre values, appreciates and acknowledges all these forces that shaped this document and this programme, and would like to extend profound and sincere thanks to all of them. A comprehensive list of all those who contributed, along with a brief history of this document, can be found in Appendix A.

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## 1 M\&S Programme Summary

## Title of the Programme

Advanced Diploma Programme in Modeling and Simulation
(the M\&S Programme for short).

## Duration of the Programme

12 months ( 48 weeks) split into 3 trimesters of 16 weeks each.

## Nature of Programme

Full time ${ }^{1}$.

## Programme Status

The M\&S programme will be run as an autonomous programme by the Centre for Modeling and Simulation, University of Pune.

## Eligibility

1. B.E. or equivalent in any branch of engineering OR Master's degree in any science, arts, or commerce discipline, AND
2. background in mathematics equivalent to the University of Pune F.Y.B.Sc. mathematics syllabus,

## Selection Criteria

1. academic record, AND
2. performance in a qualifying examination.

## Number of Seats

Not more than 30, and possibly smaller for a particular academic year.

## Total Number of Credits

48. 

## Credit Breakup

8 core courses ( 28 credits) +1 elective course ( 4 credits) + project ( 12 credits $)+$ term papers (4 credits).

## Fees

Per student fees for the entire M\&S programme: Rs. 20347 for students from the state of Maharashtra, Rs. 29147 for students from outside of Maharashtra, subject to University of Pune norms and policies as applicable.

[^0]
## 2 The M\&S Programme at a Glance

- The advanced diploma programme in modeling and simulation, also called the M\&S Programme, designed by the Centre for Modeling and Simulation, University of Pune, is a fast-paced and vigourous academic training programme that consists of core courses, an elective or specialization, term papers, and a project. The M\&S Programme uses a credit system that is manifestly compliant with the existing University of Pune credit system. One credit is thus equivalent to one clock hour of contact (between faculty and students) per week for 15 consecutive weeks, and a course could be of $1,2,3$ or 4 credits.
- This is a full-time programme. The duration of the M\&S Programme is exactly 12 months, broken up into three trimesters of 16 weeks each. The programme year should ideally and preferably start on July 1 of one academic year and end on June 30 of the next.
- The first two trimesters are devoted to coursework that consists of a total of 8 foundation (or core) courses totaling to 28 credits, plus one elective course (or specialization) of 4 credits. Each trimester is broken up into fourteen weeks of instruction, one week for exam preparations and one week for actual endtrimester examinations. Evaluation is based on (a) continuous assessment throughout the trimester, including assignments and class participation (b) final examination.
- The third trimester is devoted entirely to project work. Evaluation of the project is based on periodic monitoring of progress, a project report and a presentation cum open defense. Grade for the project component (satisfactory or otherwise) is to be mentioned separately from the grades for the rest of the programme. Students are to be encouraged to decide on and start preparing for their projects as early on in the programme as possible. The project is considered equivalent to 12 credits.
- In addition, in order to foster (a) self-study skills, resourcefulness, and independence, (b) the ability to read technical and research literature, and (c) presentation skills, a student is expected to present two term papers on topics of his or her interest and related to modeling and simulation, any time during the programme year. Evaluation of this component is to be based on (a) the term paper/report itself, and (b) the presentation. This component is considered equivalent to 4 credits.
- The credit total of the entire programme thus comes to 48 credits $=28$ (foundations) +4 (elective) +12 (project) +4 (term papers).


## 3 Introduction

This document outlines a multidisciplinary academic programme, the Advanced Diploma Programme in Modeling and Simulation, designed by the Centre for Modeling and Simulation, University of Pune. For the purpose this document, this programme may be referred to as the M\&S Programme or, simply, as the programme. The Centre for Modeling and Simulation, University of Pune, may similarly be referred to as the Centre. In this section, we present our perspective on the modeling and simulation enterprise which forms the basis for the proposed structure of the M\&S Programme.

### 3.1 The Modeling and Simulation Enterprise

Model, n. 1 a usually miniature representation of something; also : a pattern of something to be made 2 an example for imitation or emulation $\mathbf{3}$ archetype $\mathbf{4}$ a description or analogy used to help visualize something (as an atom) that cannot be directly observed 5 a system of postulates, data, and inferences presented as a mathematical description of an entity or state of affairs.
source: www.merriam-webster.com
Simulation, n. 1 The imitative representation of the functioning of one system or process by means of the functioning of another $<$ a computer simulation of an industrial process $>2$ Examination of a problem often not subject to direct experimentation by means of a simulating device.
source: www.merriam-webster.com
Simulation, n. 1 Imitation or representation, as of a potential situation or in experimental testing 2 Representation of the operation or features of one process or system through the use of another: computer simulation of an in-flight emergency 3 Attempting to predict aspects of the behaviour of some system by creating an approximate (mathematical) model of it. This can be done by physical modeling, by writing a special-purpose computer program or using a more general simulation package, probably still aimed at a particular kind of simulation (e.g., structural engineering, fluid flow). Typical examples are aircraft flight simulators or electronic circuit simulators. A great many simulation languages exist; e.g., Simula.
source: www.dictionary.com
A model tries to capture the essential features of a system under scrutiny. A simulation, on the other hand, attempts to represent a model of the system under study using some other well-understood system, the simulation system, wherein features of interest of the system under study are represented using properties of the simulation system. The correctness of representation of features of interest embodied by the model, and whether one system could at all be simulated by another should be the principal concerns of a "theory" of simulation. Assuming that the model did capture essential ingredients of the system being studied, and that the simulation
system is capable of representing the model to sufficient accuracy, the corresponding simulation could be expected to mimic the behaviour of the underlying real-life system.

Most often, mathematics is used to model the system under study. Indeed, all scientific theories can be thought of as models representing aspects of "reality" to within their own respective domains of applicability. The most challenging modeling and simulation problems arise when the system under study is neither well-understood nor, possibly, mathematised. For example, in comparison with physical systems, complex phenomena such as human social behaviour are neither as well-understood, nor are as mathematised, in microscopic detail, as physical theories. Construction of a simulation system for such phenomena may have somewhat nebulous boundaries between an art and a science. Further, validity bounds of the mathematical theory used in constructing the underlying mathematical model for a system has a direct influence on the reliability of the simulation system. The degree of identity (or similarity) between the behaviour of the real system and the simulated system needs to be determined so as to enable making of valid inferences based on observations of the simulated system.

A mathematical model typically extracts essential features of the system under study from the knowledge domain. For example, the mathematical model of air flight would have to incorporate fluid dynamical statements about the properties of air as a fluid system. A typical modern scientific team working on a challenging real-life problem consists of domain experts (e.g., experts in fluid dynamics), mathematical modeling experts, and experts from the field that is being used to construct the simulation system. In case modern digital computers are used to perform a simulation, the field of expertise for constructing a simulation system would be computer science and engineering. Other cases, for example, a full-scale flight simulation system, could involve expertise from almost every branch of engineering and robotics just to construct the simulation system.

A simulation is thus built using these three principal components; namely, (a) domain expertise, (b) mathematical modeling strategies, and (c) simulation system methodologies (including technology).

In modern times, digital computers have emerged as the preferred simulation system to perform simulations on. Usually, a mathematical model of the system under scrutiny is programmed into a computer and then run, and the behaviour of the model as observed in this simulation is used to make inferences about the real system that is being modeled and simulated. It appears that the use of computers saves costs because employing them in place of full-scale physical simulation systems reduces the engineering overheads (although the scientific principles at the base still need to be incorporated).

If we choose to use a computer to perform simulations, then its behaviour and properties as a simulation system must be "well-understood": this implies that an academic programme designed around the use of computers as simulation systems of choice must have sufficient theoretical and practical content to ensure strong foundations in computation.

### 3.2 Need for a Programme in Modeling and Simulation

The rapid pace of advances in computer and computation-related technologies over last few decades and the ever-increasing availability of comparatively inexpensive raw computing power have encouraged the use of computation in general, and simulation methods in particular, wherever quantitative reasoning has a significant role to play. This includes all branches of the scientific and technological endeavour.

Typical degree programmes (such as a two-year Masters programme in physical sciences mathematics and statistics, or Bachelors/Masters programmes in an engineering discipline) often include an introductory course on programming, and perhaps another one on domain-specific computational methods. Nevertheless, a sound foundation in all three aspects of modeling and simulation is usually impossible to develop during such courses given the constraints and workload of a typical degree programme.

The M\&S Programme designed by the Centre hopes to fill the gap between (a) a conventional degree programme and a research (Ph.D.) programme involving extensive computational and simulational research, and (b) a conventional degree programme and industrial R\&D work requiring substantial background in modeling and simulation. From another perspective, the M\&S Programme is geared to create a breed of problem solvers with a breadth and perspective on modeling, good training in simulation methods, and the ability to generate reasonable solutions for problems not necessarily encountered previously.

## 4 Programme Design Considerations

### 4.1 From an Academic Perspective

As we saw earlier, a simulation is built on

- domain expertise,
- mathematical modeling strategies, and
- simulation system methodologies (including technology).

An advanced diploma programme such as the present one may be designed such that at the successful completion of training, a student may be one of the following:

1. Conversant with the basic principles in all the three components, or
2. Conversant with basic principles in the mathematical and simulational components, but unaware of any domain expertise, or
3. Conversant with only the simulational components, but unaware of domain expertise and mathematical methods, or
4. Be skilled, as opposed to conversant, with the basic principles of all the three components, but be aware/conversant with a few advanced techniques from the three, or
5. Be skilled, as opposed to conversant, with the basic principles of mathematical and simulational components, but be aware/conversant with a few techniques from the first, or
6. Be skilled, as opposed to conversant, with the basic principles of simulational components, but be aware/conversant with a few techniques from the first and the second ${ }^{2}$.

All possibilities other than those above are intuitively judged to be more intensive and hence most likely to be out of the time bound of a one-year programme. (1)(3) have been included because given that the proposed course is a post-graduate diploma course, it may find favour to be licensed to outside entities for a wider spread $^{3}$. (4)-(6) are a set of levels of decreasing intensity, but admissible for a University post-graduate diploma course spanning 12 months. The alternative (4) is the most intense one, requiring active involvement of experts in all the three components, thus unsuitable for operation by the Centre in its current state.

Alternative (5) is the most practical alternative for the M\&S Programme; we have thus proposed a course structure based on this alternative. Nevertheless, we would like to build provisions into the programme structure to offer specialized expert-level courses as and when domain experts become available.

### 4.2 From a Student's Perspective

A typical candidate looks at a degree or a diploma from the point of view of job prospects and at a diploma as a value addition. Employment opportunities for a graduate of the M\&S Programme are most likely to come from:

- Research programmes leading to an advanced degree such as Ph.D.
- Research-oriented support positions in research institutions.
- Industries and organizations that require simulation-based methodologies.


## 5 Objectives and Outcomes

Assuming that alternative (5) in Section 4.1 is the way to go, then at the end of the diploma, we expect that a graduate of the $M \& S$ Programme to be the following:

- A problem solver with a breadth and perspective on modeling, good training in computation and simulation methods, and the ability to generate reasonable solutions for problems not necessarily encountered earlier.

[^1]- Outside of his or her knowledge domain, (s)he is able to create a computer representation of a specific detailed description of the problem domain given that a domain expert has distilled the computational essence for him or her.
- Familiar with the current state of relevant technologies, and from familiar to skilled in a variety of relevant software tools and methodologies.


## 6 The Prospective Student

### 6.1 Prerequisites

Structure of the M\&S Programme is built around the assumption that a prospective student satisfies these three principal prerequisites:

- At least a Bachelor's degree in an engineering discipline OR a Masters degree in a science, commerce or arts discipline, AND
- A demonstrable background in mathematics at the level of the current University of Pune first-year B.Sc. mathematics syllabus (to be assessed via a qualifying (or entrance) examination (see Section 6.2) and the academic record), AND
- Basic computer usage skills (to be assessed via a qualifying (or entrance) examination (see Section 6.2) preferably with some programming experience.


### 6.2 Selection

Students will be selected on the basis of

1. academic record,
2. qualifying (or entrance) examination, and
3. statement of purpose.

The qualifying (or entrance) examination will be designed to test basic analytical and reasoning skills, mathematics background, and computer literacy. Passing threshold for the qualifying (or entrance) examination will be at $60 \%$ for both (open and reserved) categories. The Centre will select not more than 30 top-scoring candidates consistent with University norms on reservation.

## 7 Academic Structure

The M\&S Programme consists of the following four components. Section 7.1 presents our outlook (in the design) and guidelines (for conducting the M\&S programme).

1. Foundation (or Core) Courses (Section 7.2).
2. Elective (Section 7.3).
3. Project (Section 7.4).
4. Term Papers (Section 7.5).

### 7.1 Outlook and Guidelines

Given the highly multidisciplinary, vigourous and compact nature of the M\&S Programme, we find it highly essential to adopt the following outlook in designing the proposed course work (these would serve as the essential guidelines when running the M\&S programme):

- Rigour and clarity are not always synonymous: concepts need to be emphasized from a practical and application standpoint in place of tedious derivations and rigourous proofs.
- It is highly essential to impart to the students a perspective on modeling and simulation that will bring together this diverse set of concepts into a unified view, both from conceptual and practical points of view.
- The role of well-chosen and well-motivated students, well-designed instruction material, effective presentation methods, and ready availability of academic and computational resources relevant to the M\&S programme cannot be overemphasized.
- See Section 7.6 for guidelines on evaluation and grading.


### 7.2 The Foundations

Essential basics for a programme on modeling and (computational) simulation should come from applied mathematics (includes probability theory and statistics) on one hand and the theory of computation on the other. The essential methodologies required for a computational simulation are simulation methods and software techniques. This justifies the following five-fold logical structure for the foundations of modeling and simulation:

## 1. Core Mathematics

2. Theory of Computation
3. Perspectives on Mathematical Modeling
4. Perspectives on Probability Modeling
5. Practical Computing: Technologies and Methodologies

In the rest of this section, we expand this logical structure into a set of 8 foundational courses of the M\&S Programme, detailed syllabi of which appear in Appendix B.

### 7.2.1 Core Mathematics

Rationale and Outlook - This group of modules serves to (a) establish a common denominator for mathematical training keeping in mind the students' diverse and nonuniform mathematical training, (b) equip the student to read through, and to be able to grasp, elementary mathematical treatments of specialized topics, and (c) cover common mathematics prerequisites of other modules.

Module

- Essentials of Analysis
- Linear Algebra
- Discrete Mathematics
- Probability Theory and Stochastic Processes


## Syllabus <br> Section

## B.1.1

B.1.2
B.1.4
B.1.3
Total Number of Contact Hours 60
Total Number of Credits 4

### 7.2.2 Theory of Computation

Rationale and Outlook • This group of modules is designed (a) to expose the student to various aspects of the fundamental question "what is computation?", (b) to introduce formal aspects of programming and of algorithm design and analysis, and (c) to introduce a formalism that has a potentially wide applicability as a formalism for modeling: Two known examples of such modeling contexts outside of conventional computer science home grounds, where, e.g., theory of formal languages has a high utility are analysis of complex systems (characterization of complexity, symbolic dynamics of dynamical systems), and sequence analysis in bioinformatics.

Module
Syllabus
Section

- Theory of Computation
B.2.1
- Programming: Theory and Perspectives B.2.2
- Algorithm Design and Analysis
B.2.3

Total Number of Contact Hours 60
Total Number of Credits 4

### 7.2.3 Perspectives on Mathematical Modeling I

Rationale and Outlook - The utility of applied mathematics as a formalism for modeling needs no justification. This group of modules is intended to cover areas of
applied mathematics most commonly encountered in modeling and simulation contexts.

In order to emphasize the modeling perspective and maintain focus on applications, we suggest a three-component structure for each of these modules; this structure consists of: (a) basic theory and pertinent mathematical results, (b) perspective on modeling by way of real-life contexts, examples and applications, and (c) relevant numerical methods.

$$
\text { Module } \begin{gathered}
\text { Syllabus } \\
\text { Section }
\end{gathered}
$$

- Modeling Change with Difference Equations B.3.1
- Ordinary Differential Equations, Dynamics and Nonlinearity B.3.2
- Partial Differential Equations and Finite Element Methods B.3.3
- Integral Equations B.3.4
- Calculus of Variations B.3.5
$\begin{array}{lr}\text { Total Number of Contact Hours } & 60 \\ \text { Total Number of Credits } & 4\end{array}$


### 7.2.4 Perspectives on Mathematical Modeling II

Rationale and Outlook - Same as that of Section 7.2.3.

Module
Syllabus
Section

- Transforms
B.4.1
- Optimization
- Numerical Linear Algebra: A User's Perspective
- Miscellaneous Topics in Numerical Analysis
B.4.2
B.4.3
B.4.4

Total Number of Contact Hours 60
Total Number of Credits 4

### 7.2.5 Perspectives on Probability Modeling I

Rationale and Outlook - Probability is the mathematical language for quantifying uncertainty or ignorance, and is the foundation of statistical inference and all probability-based modeling. Assuming a background in probability theory (developed as a Core Mathematics module, Section 7.2.1), this course introduces the basics of statistical inference and probabilistic methods in modeling and simulation.

In order to emphasize the modeling perspective and maintain focus on applications, we suggest a three-component structure for each of these modules; this structure consists of: (a) basic theory and pertinent mathematical results, (b) per-
spective on modeling by way of real-life contexts, examples and applications, and (c) relevant numerical methods.

Module Syllabus
Section

- Reasoning Under Uncertainty B.5.1
- Stochastic Simulation B.5.2
- Stochastic Differential Equations B.5.3

Total Number of Contact Hours 45
Total Number of Credits 3

### 7.2.6 Perspectives on Probability Modeling II

Rationale and Outlook • Same as that of Section 7.2.5.
Module
Syllabus
Section

- Statistical Models and Methods
- Stochastic Optimization
B.6.1
B.6.2

Total Number of Contact Hours 45

### 7.2.7 Practical Computing I

Rationale and Outlook - A solid background in basic software methodologies and technologies together with ample hands-on experience is highly necessary to be able to effectively utilize the perspective in modeling and simulation that are developed through the rest of the M\&S programme.
Module
Syllabus
Syllabus
Section

- Truncated Numbers and Finite-Precision Arithmetic ..... B.7. 1
- Systems Modeling and Simulation ..... B.7.2
- Programming Paradigms and Perspectives Hands-On ..... B.7.3
- Case Studies I ..... B.7.4
Total Number of Contact Hours ..... 45
Total Number of Credits ..... 3


### 7.2.8 Practical Computing II

Rationale and Outlook • Same as that of Section 7.2.7.
Module Syllabus

- High-Performance Computing B.8.1
- Case Studies II B.8.2

Total Number of Contact Hours 45
Total Number of Credits 3

### 7.3 Electives

Rationale and Outlook • Given the preparation of the first two trimesters and the core courses, a student is expected to be in a position to assimilate material from advanced, specialized, or domain-specific elective modules of his or her choice ${ }^{4}$. These elective modules are expected to demonstrate applications of the concepts developed towards the construction of real simulations.

In this section, we simply list a number of possibilities for the electives; detailed syllabi will be developed as and when required:

- Simulations in Physics
- Materials and Molecular Modeling
- Introduction to M\&S for Complex Systems
- Six Degrees of Separation: an Introduction to Networks
- Evolutionary and Agent-Based Modeling
- Quantum Computing
- Digital Signal Processing
- Monte Carlo Methods in Finance
- Neural Networks, Machine Learning and Data Mining

The elective is one full course ( 4 credits):
Total Number of Contact Hours 60
Total Number of Credits 4

[^2]
### 7.4 The Project

Rationale and Outlook • Given the highly applied nature of the M\&S Programme, it is natural to emphasize substantial hands-on project work. We thus propose

- to use an acceptability criterion for project work that is much higher than the standard University of Pune passing grade of $\mathrm{C}+$.
- that project grade should be mentioned separately from the GPA for the rest of the course.
- that students be encouraged to look for and start preparing for their projects as early on during the M\&S Programme as possible.

The project is considered equivalent to 3 full courses or 12 credits:
Total Number of Contact Hours 180
Total Number of Credits 12

### 7.5 The Term Papers

Rationale and Outlook • In addition, in order to foster self-study skills, resourcefulness, independence, plus the ability to read technical and research literature and make presentations, a student is expected to present two term papers on a topic of his or her interest related to modeling and simulation. Evaluation of the term papers will be based on (a) the term paper/report itself, and (b) a presentation. The term papers are considered equivalent to 1 full course or 4 credits:

Total Number of Contact Hours 60
Total Number of Credits 4

### 7.6 Evaluation and Grading

We recommend the following guidelines for student evaluation:

1. Adequate weightage to both "theory" and "practice" aspects.
2. Continuous evaluation throughout a programme year that aims at accurately assessing the knowledge, abilities and skills relevant to modeling and simulation acquired through the M\&S programme. This may include, at the discretion of an instructor, class participation.
3. Periodic examinations consistent with existing University of Pune practices and patterns, yet designed to bring about the real knowledge, abilities and skills of a student.

## A History and Credits

- An initial draft of this document emerged in mid-2004 out of close interactions, uncountable informal discussions, unique individual perspectives, and several formal meetings, between members of a core group at the Center for Modeling and Simulation (in reverse-alphabetical order: Vaishali Shah, Ajay Nandgaonkar, Sailaja Krishnamurty, D. G. Kanhere, P. M. Gade, Mihir Arjunwadkar) and two experts closely associated with the Centre (Abhijat Vichare, CFDVS, IIT Powai, and Ashutosh, Agilent Systems Pvt. Ltd., Pune).
- Abhijat Vichare, in particular, deserves a major part of the credit for defining and refining our outlook on simulation and modeling, and for contributing his own version of this document, parts of which have been incorporated almost verbatim in this document.
- Those who contributed syllabi for topics of their specialty or choice (in reversealphabetical order) are: Abhijat Vichare, Anagha Kuvalekar, Neeta Kshemkalyani, Sailaja Krishnamurty, P. M. Gade, Ashutosh, and Mihir Arjunwadkar. These have been incorporated in this proposal without alteration.
- In the process of designing the syllabi, some of us have consulted many online resources on the web, some of which have been cited under individual syllabi. The rest are too numerous to list: we acknowledge these with sincere thanks.
- Mihir Arjunwadkar coordinated the entire development of the M\&S programme and the evolution this document.
- This document was sent for review and feedback to experts both from academics and industry. Those who responded and shared their views and insights with us are listed below, with our sincere thanks, in a reverse-alphabetical order:

Abhijat Vichare (CFDVS, IIT Powai) • William Sawyer (Department of Environmental Sciences, ETH Zürich) • R. Sankarasubramanian (Defense Materials Research Laboratory, Hyderabad) - Mangesh Patwardhan (National Insurance Academy, Pune) • Abhay Parvate (Department of Physics, University of Pune) • Suhas Pansare (KPIT Pvt. Ltd., Pune) • Uttara NaikNimbalkar (Department of Statistics, University of Pune) • Rustom Mody (Department of Computer Science, University of Pune) - Subhash Ghaisas (Department of Electronic Sciences, University of Pune) • Anil Gangal (Department of Physics, University of Pune) - Ashutosh (Agilent Systems, Pvt. Ltd., Pune)

## B Syllabus

1 We assume that the reader, at this point, is already familiar with all of the preceding sections of this document. The reader may, however, find it useful to refer to Section 7.1 that outlines our academic outlook, to Section 7.2 that provides an outline with justification for the modulewise syllabi provided in this section, and to Section 1 and 2 that summarize the entire M\&S Programme in a succinct manner.

2 Here is the credit break-up for the entire $M \& S$ programme, plus a roadmap into this document:

| M\&S Programme Component | Credits | Main Document <br> Section | Syllabus <br> Section |
| :--- | :---: | :---: | :---: |
| - Foundational (Core) Courses | 28 | $7.2 .1-7.2 .8$ | B.1-B.8 |
| - Elective | 4 | 7.3 | B.9 |
| - Project | 12 | 7.4 | B.10 |
| - Term Papers | 4 | 7.5 | B.11 |

Total Number of Programme Credits 48
3 The actual order of presentation of individual modules below to the students would need to take into account modulewise dependencies and prerequisites.

4 Course codes assigned in this section are tentative at this stage. They are of the form CMS-M\&S-t-c, where $t$ indicates the trimester in which the course is to be run, and $c$ indicates, for the core courses, the course number under Section 7.2.

## B. 1 Core Mathematics (CMS-M\&S-1-1)

## B.1.1 Essentials of Analysis

Number of Lectures • 5
Prerequisites • None
Syllabus
Review of real analysis, (continuity, differentiability, limits of sequences and functions, integration)

Complex numbers, complex functions, limits and continuity Complex differentiation, analytic and harmonic functions, Complex integration, Line integrals, Cauchy theorem, Cauchy integral formula, Residues and applications, Taylor and Laurent series. Elementary overview of branch cuts(?).

## Suggested Texts and References

R. V. Churchill- Complex variables and Applications, 7th Ed. McGraw Hill.

## B.1.2 Linear Algebra

Number of Lectures • 20
Prerequisites • None
Syllabus

1. Linear Equations. Introduction. Gaussian elimination and matrices. GaussJordan method. Two-point boundary-value problems. Making gaussian elimination work. Ill-conditioned systems.
2. Rectangular Systems and Echelon Forms. Row echelon form and rank. The reduced row echelon form. Consistency of linear systems. Homogeneous systems. Nonhomogeneous systems. Electrical circuits.
3. Matrix Algebra. Addition, scalar multiplication, and transposition. Linearity. Why do it this way. Matrix multiplication. Properties of matrix multiplication. Matrix inversion. Inverses of sums and sensitivity. Elementary matrices and equivalence. The LU factorization.
4. Vector Spaces. Spaces and subspaces. Four fundamental subspaces. Linear independence. Basis and dimension. More about rank. Classical least squares. Linear transformations. Change of basis and similarity. Invariant subspaces.
5. Norms, Inner Products, and Orthogonality. Vector norms. Matrix norms. Inner product spaces. Orthogonal vectors. Gram-Schmidt procedure. Unitary and orthogonal matrices. Orthogonal reduction. The discrete fourier transform.

Complementary subspaces. Range-nullspace decomposition. Orthogonal decomposition. Singular value decomposition. Orthogonal projection. Why least squares? Angles between subspaces.
6. Determinants. Properties of determinants.
7. Eigenvalues and Eigenvectors. Elementary properties of eigensystems. Diagonalization by similarity transformations. Functions of diagonalizable matrices. Systems of differential equations. Normal matrices. Positive definite matrices. Nilpotent matrices and Jordan structure. The Jordan form. Functions of non-diagonalizable matrices. Difference equations, limits, and summability. Minimum polynomials and Krylov methods.
8. Perron-Frobenius Theory of Nonnegative Matrices. Introduction. Positive matrices. Nonnegative matrices. Stochastic matrices and Markov chains.

## Suggested Texts and References

- Matrix Analysis and Applied Linear Algebra, Carl D. Meyer, Society for Industrial and Applied Mathematics (SIAM) (2000). Available as a public web resource at http://www.matrixanalysis.com/.


## B.1.3 Probability Theory and Stochastic Processes

Number of Lectures - 20
Prerequisites • B.1.4(1,2)

## Syllabus

1. Probability. Sample spaces and events. Probability on finite sample spaces. Independent events. Conditional probability. Bayes' theorem.
2. Random Variables. Distribution functions and probability functions. Important discrete and continuous random variables. Bivariate and multivariate distributions. Independent random variables. Conditional distributions. Important multivariate distributions. Transformations on one or more random variables.
3. Expectation. Properties. Variance and covariance. Expectation and variance for important random variables. Conditional expectation. Moment generating functions.
4. Inequalities for Probabilities and Expectations.
5. Convergence and Limit Theorems. Notion of convergence for random variables. Types of convergence. Law of large numbers, central limit theorem, the delta method.
6. Stochastic Processes. Simple branching processes and random walks. Markov chains in discrete time. Poisson processes and renewal theory. Point processes. Continuous-time Markov processes. Birth and death processes.

## Suggested Texts and References

- Elementary Probability, David Stirzacker, Cambridge University Press (1994). Indian edition/reprint available.
- Probability and Random Processes, Geoffrey R. Grimmett and David R. Stirzacker, Oxford University Press (2001).
- All of Statistics, Larry Wasserman, Springer-Verlag (2004).


## B.1.4 Discrete Mathematics

Number of Lectures • 15
Prerequisites • None

## Syllabus

1. Sets. Sets, subsets, counting subsets, power set, finite and infinite sets, cardinality. Operations on sets: union and intersection, difference and symmetric difference, cartesian product. Cardinality of a union and the inclusionexclusion principle. Cardinality of a cartesian product. Tree diagrams. Partition of a set. Characteristic function of a set. Multisets.
2. Fundamental Notions of Mathematics. Definitions, axioms, propositions, logical deductions, proofs, counterexamples. Boolean algebra and its relationship with predicate and propositional calculi. Good proofs and bad proofs. Proof techniques: induction, contradiction, pigeonhole principle. Induction axiom and examples. Strong induction. Induction, strong induction and the least number principle.
3. Relations. Properties of relations. Representations: lists, Boolean matrices, diagraphs. Operations on relations: inverse, composition, closure; reflexive, symmetric and transitive closures; computing the transitive closure. Equivalence relations.
4. Partially Ordered Sets. Partial orders as directed acyclic graphs. Partial vs. total orders. Topological sorting. Chains, Dilworth's theorem, increasing and decreasing sequences. Analysis of the parallel task scheduling problem.
5. Assorted Notation. Sum, factorial, product. Assorted examples: finite and infinite geometric series and related sums, harmonic numbers and series, Stirling approximation. Asymptotics: big $O$, little $o, \Omega$ and $\Theta$. Pitfalls with big $O$. floor and ceiling.
6. Functions, Counting, Pigeonholing, Permutations. Functions, domain and image, inverse functions; composition, identity functions; bijections, injections, surjections. Counting functions. The pigeonhole principle and Cantor's theorem. Permutations, cycle notation, transpositions. Application: lower bound for sorting. $r$-permutations. Division rule. Combinations. r-combinations.

Binomial and multinomial coefficients. $r$-permutations and $r$-combinations with repetition and limited repetition. Assorted examples and applications. Hall's marriage theorem.
7. Graphs. Simple graphs, multigraphs, directed graphs, weighted graphs. Realworld examples. Graphs isomorphism. Properties of graphs: vertex degree, chromatic number, paths in graphs, adjacency matrices, connectedness. Trees. Eulerian graphs.
8. More on Induction. Applications of induction and other proof techniques to analysis of algorithms. Recursive definitions and structural induction.
9. Elementary Number Theory. Division, greatest common divisor, modular arithmetic, chinese remainder theorem, factoring, Fermat's little theorem, Euler's theorem.
10. Groups and Other Algebraic Structures. Semigroups, groups, group isomorphism, cyclic groups, subgroups, Lagrange's theorem. Symmetry and symmetry groups, symmetries as permutations, combining symmetries. Monoids, fields, rings, lattices, etc.

## Suggested Texts and References

- Mathematics-A Discrete Introduction, Edward R. Scheinerman, Brooks/Cole Publishing Company (2000). Indian edition/reprint available.
- Discrete Mathematics, Seymor Lipschutz and Marc Lipson, Schaum's Outline Series, McGraw-Hill (second edition, 1997).
- Mathematics for Computer Science. Available as a public web resource at http://aka-ocw.mit.edu/OcwWeb/Electrical-Engineering-and-Computer-Science/6-042JMathematics-for-Computer-ScienceFall2002/CourseHome/index.htm.


## B. 2 Theory of Computation (CMS-M\&S-1-2)

## B.2.1 Theory of Computation

Number of Lectures • 20
Prerequisites • B.1.4

## Syllabus

1. Introduction to Languages. Symbols, strings, words and languages. Symbolic Dynamics, dynamics as language. Examples of languages. Finite representation of languages. String induction principles.
2. Finite Automata. Functions as tables: introduction to theory of automata. Regular expressions and languages. Equivalence and simplification of regular expressions. Finite automata and labeled paths. Isomorphism of finite automata. Algorithms for checking acceptance and finding accepting paths. Simplification of finite automata. Proving the correctness of finite automata. Empty-string/Nondeterministic/Deterministic
3. Context-Free Grammers. Examples of languages which are not regular. State minimization. The pumping lemma for regular languages. Context-free grammars, parse trees, stacks and queues. Dynamical systems generating contextfree languages. Functions with "internal memory" and push-down automata. Converting between parse trees and derivations. Simplification and ambiguity of grammars. Determinism and parsing. Pumping lemma for context free grammars.
4. Turing Machines. Examples which are not context free. Chomsky hierarchy. Another look at symblic dynamics and coding theory for examples of dynamical systems in various levels of chomsky hierarchy. Computing with dynamical systems. Functions with "external memory" and Turing machines.

## Suggested Texts and References

- Elements of Theory of Computation, H. Lewis and C. Papadimitrion, PrenticeHall (second edition, 1998).
- Introductory Theory of Computer Science, V. E. Krishnamurthy, Gage Distribution Co. (1983) and Springer-Verlag (1985). Indian edition/reprint available.
- Feynman Lectures on Computation, R. P. Feynman, Perseus Books Group (2000).


## B.2.2 Programming: Theory and Perspectives

Number of Lectures • 25
Prerequisites • None

## Syllabus

1. Programming Languages Inroduction. Programming linguistics. Concepts and paradigms. Syntax, semantics, and pragmatics. Language processors. Historical development.
2. Basic Concepts. Primitive, Composite, Recursive types. Expressions (Conditional, Iterative). Literals. Function calls. Variables and Storage. Copy semantics vs. reference semantics. Lifetime. Global and local variables. Pointers. Bindings and Scope. Declarations Procedural Abstraction .
3. Advanced Concepts. Data Abstraction. Encapsulation. Abstract types. Objects and classes. Generic Abstraction. Polymorphism. Overloading. Control Flow. Concurrency.
4. Paradigms. Imperative Programming; case study: Ada. Object-Oriented Programming; case study: C++. Concurrent Programming. Java. Functional Programming; case study: Lisp. Logic Programming; case study: Prolog. Scripting; case study: Python and Perl.
5. Language Selection. Criteria. Evaluation.

## Suggested Texts and References

- Program Style, Design, Efficiency, Debugging and Testing, D. Van Tassel, Prentice-Hall (1978).
- Structure and Interpretation of Computer Programs Harold Abelson, Gerald Jay Sussman and Julie Sussman, The MIT Press (2nd edition, 1996). Available as a public web resource at http://www-mitpress.mit.edu/sicp/full-text/book/book.html.
- Programming Languages: Principles and Paradigms, Allen B. Tucker, Robert Noonan McGraw-Hill (2002).
- Programming Language Concepts and Paradigms, David A. Watt, PrenticeHall (1990).
- Programming Language Design Concepts, David A. Watt, John Wiley and Sons, Inc. (2004). Available as a public web resource at http://www.dcs.gla.ac.uk/~daw/books/PLDC/index.html.


## B.2.3 Algorithm Design and Analysis

Number of Lectures • 15
Prerequisites • None

## Syllabus

1. Algorithm Analysis. Methodologies for Analyzing Algorithms. Asymptotic Notation.
2. Basic Data Structures. Stacks and Queues. Vectors, Lists, and Sequences. Trees. Priority Queues and Heaps. Dictionaries and Hash Tables.
3. Search Trees. Ordered Dictionaries and Binary Search Trees. AVL Trees. Bounded-Depth Search Trees.
4. Sorting. Merge-Sort. Quick-Sort. A Lower Bound on Comparison-Based Sorting. Bucket-Sort. Comparison of Sorting Algorithms.
5. Fundamental Techniques. The Greedy Method. Divide-and-Conquer. Dynamic Programming.
6. Graphs. Graph Traversal. Directed Graphs. Depth-First Search. Weighted Graphs. Single-Source Shortest Paths. All-Pairs Shortest Paths. Minimum Spanning Trees.
7. Network Flow and Matching. Flows and Cuts. Maximum Flow. Maximum Bipartite Matching. Minimum-Cost Flow.
8. NP-Completeness. P and NP. NP-Completeness. Important NP-Complete Problems. Approximation Algorithms. Backtracking and Branch-and-Bound.

## Suggested Texts and References

- Design and Analysis of Algorithms, A. V. Aho, J. E. Hopcroft and J. D. Ullman, Addison-Wesley (1976).
- Fundamentals of Computer Algorithms, E. Horowitz, S. Sahni, Galgotia Publishers (1984).


## B. 3 Perspectives on Mathematical Modeling I (CMS-M\&S-1-3)

## B.3.1 Modeling Change with Difference Equations

Number of Lectures • 7
Prerequisites • B.1.1
Syllabus

1. Introduction. Sequences and differences. Properties and applications of difference tables.
2. Modeling Change with Difference Equations. Perspective from applications in mechanics, population growth, population genetics, macroeconomics, ...
3. Solving Linear Homogeneous Difference Equations. Nonhomogeneous linear difference equations. Discrete transforms in the solution of linear difference equations.
4. First-Order Nonlinear Difference Equations.
5. Systems of Difference Equations.
6. Sums and Series.
7. Transition to Calculus. Difference equations to differential equations.

## Suggested Texts and References

- Modelling with Differential and Difference Equations, Glenn Fulford, Peter Forrester and Arthur Jones, Cambridge University Press (1997). ISBN 052144618X.
- Difference Equations to Differential Equations: An Introduction to Calculus, Dan C. Sloughter. Available as a public web resource at http://math.furman.edu/~dcs/book/.
- Linear Difference Equations with Discrete Transforms Method, Abdul J. Jerri, Kluwer Academic Publishers (1996). ISBN 0792339401.

Module contributed by Mihir Arjunwadkar

## B.3.2 Ordinary Differential Equations, Dynamics and Nonlinearity

Number of Lectures • 20
Prerequisites • None

## Syllabus

Autonomous and non-autonomous first and second order non-linear differential equations (ie. vector fields), deterministic, stochastic...physical examples. Phase space, stability analysis, Poincare sections.

Linear and non-linear difference equations (ie. Maps), logistic, area preserving, Henon, Chirikov, routes to chaos, period doubling, quasiperiodicity and intermittency. Lyapunov exponent. Definition and numerical calculation.

Strange attractors (Quantifiers: Fractal dimension, topological entropy, information entropy).

Suggested Texts and References
E. Ott, Chaos in Dynamical Systems, (Cambridge, Second Ed. 2002 )
S.H. Strogatz, Nonlinear Dynamics and Chaos, (Addison-Wesley 1994)

Module contributed by P. M. Gade

## B.3.3 Partial Differential Equations and Finite Element Methods

Number of Lectures • 20
Prerequisites • None
Syllabus

1. Parabolic Equations in One Space Variable. Explicit schemes: notations, trunctation error, convergence. An implicit method. More general boundary conditions. Prabolic equations in two and three dimesions. ADI method in two and three dimensions. Curved boundaries. Application to general parabolic problems.
2. Hyperbolic Equations in One Space Dimension. Characterisitcs. The CFL condition. Error analysis of the upwind scheme. Comparision of phase and amplitude analysis. Consistency, convergence and stablity. Hyperbolic equations in higher dimensions.
3. Elliptic Equations in One, Two and Three Space Dimensions.
4. Additional Topics. Rigorous convergence analysis. Matrix method for stability analysis and spectral methods.

## Suggested Texts and References

- Beginning Partial Differential Equations, P. V. O’Neil, John Wiley and Sons Inc. (1999).
- Differential Equations with Applications and Historical Notes, G. F. Simmons, McGraw-Hill (1993).


## B.3.4 Integral Equations

Number of Lectures • 7
Prerequisites • None

## Syllabus

Integral equations, Fredholm integral equation of first kind, Fredholm integral equation of second kind, Volterra integral equation of first kind, Voltera integral equation of second kind, applications.

Suggested Texts and References
Arfken, G. "Integral Equations." Ch. 16 in Mathematical Methods for Physicists, 3rd ed. Orlando, FL: Academic Press, pp. 865-924, 1985.

## B.3.5 Calculus of Variations

Number of Lectures • 6
Prerequisites • B.1.1, B.1.2
Syllabus

1. Basics of Calculus of Variations.
2. Elements of Functional Analysis.
3. Applications in Mechanics and Optimal Control Theory.

## Suggested Texts and References

- The Calculus of Variations and Functional Analysis, Leonid P. Lebedev and Michael J. Cloud, World Scientific (2003).


## B. 4 Perspectives on Mathematical Modeling II (CMS-M\&S-2-4)

## B.4.1 Transforms

Number of Lectures • 20
Prerequisites • None
Syllabus
Fourier transform. Wiener-Khinchin theorem. Fast Fourier Transform. Applications

Laplace transform. Laplace transforms of simple functions. Applications to solving differential equations.

Wavelet transform. Definition and applications.
Radon transform, Hough transform. Basic theory and applications.
Hilbert Transform.
An introduction to some other useful transforms. More emphasis on applications and salient features of different transforms which make them applicable in different cases. Less emphasis on proofs. However, student should be able to derive simple properties of transforms.

Suggested Texts and References
Boggess and Narcowich, A First Course in Wavelets with Fourier Analysis, Prentice Hall, 2001

Walnut, David F., An Introduction to Wavelets Analysis, Birkhauser Boston, 2001,
L. C. Andrews and B. K. Shivamoggi, Integral Transforms for Engineers, (PrenticeHall of India, 2003)

## B.4.2 Optimization

Number of Lectures • 20
Prerequisites • None
Syllabus

1. Optimization. Basic ingradients. Classification of optimization problems.
2. Convex Optimization. Mathemetics of convex optimization problems. KuhnTucker theorem. Duality. Linear optimization. Simplex methods. Conic optimization. Non-linear optimization. Application: use of Simplex method in determining the solvations sites in a protein model.
3. Unconstrained Optimization. Decent methods. Gradient-based methods. Newton and quasi-newtons methods. BFGS method. Methods without derivatives.
4. Constrained Optimization. Equality constraints. Quadratic programming. Methods of feasible directions. Linearizion method. Inequality constraints and a Theorem due to Kuhn and Tucker.
5. Discreate Optimization. Linear and integer optimization. Semi-definite programming. Graph algorithms. Geometric algorithms. Applications to the real world.
6. Non-Convex Optimization. Branch and bound methods for nonconvex optimization. Convexing a non-convex optimization. Heuristic methods for nonconvex optimization.

## Suggested Texts and References

- Numerical Methods in Extremal Problems, B. N. Pshenichny and Yu. M. Danilin, MIR Publications, Moscow (1978).
- A First Course in Optimization Theory, R. K. Sundaram, Cambridge University Press (1996). ISBN 0521497701. Associated website: http://www.cambridge.org/us/catalogue/catalogue.asp?isbn=0521497701.
- Optimization Theory with Applications, D. A. Pierre, Dover (1986). ISBN 048665205X.
- An Introduction to the Conjugate Gradient Method Without the Agonizing Pain, Jonathan Richard Shewchuck, Carnegie Mellon School of Computer Science Techincal Report CS-94-125 (1994). Available as a public web resource at http://historical.ncstrl.org/tr/ps/cmucs/CMU-CS-94-125.ps.

Module contributed by Sailaja Krishnamurty

## B.4.3 Numerical Linear Algebra: A User's Perspective

Number of Lectures • 15
Prerequisites - B.1.2, B.7.1

## Syllabus

1. Matrix Multiplication Problems. Basic algorithms. Exploiting structure: algorithms for band and sparse matrices. Vectorization and reuse issues.
2. The Basics. Review of basic ideas from linear algebra. Vector and matrix norms. Finite precision issues. Orthogonality and the SVD. Projections and the CS decomposition. Sensitivity of square linear systems.
3. General Linear Systems. Triangular systems. LU factorization. Roundoff analysis of Gaussian elimination. Pivoting. Improving and estimating accuracy.
4. Special Linear Systems. $\mathrm{LDM}^{T}$ and $\mathrm{LDL}^{T}$ factorizations. Positive definite systems. Banded systems. Symmetric indefinite systems. Block systems. Vandermonde systems and the FFT. Toeplitz and related systems.
5. Orthogonalization and Least Squares. Householder and Givens matrices. QR factorization. Full-rank LS problem. Other orthogonal factorizations. Rankdeficient LS problem. Weighing and iterative improvement. Square and underdetermined systems.
6. Parallel Matrix Computations. Basic concepts. Matrix multiplication. Factorizations.
7. The Unsymmetric Eigenvalue Problem. Properties and decompositions. Perturbation theory. Power iterations. Hessenberg and Real Schur forms. The practical QR algorithm. Invariant subspace computations. The QZ method for $A x=\lambda B x$.
8. The Symmetric Eigenvalue Problem. Properties and decompositions. Power iterations. The symmetric QR algorithm. Jacobi methods. Tridiagonal methods. Computing the SVD. Generalized eigenvalue problems.
9. Lanczos Methods. Derivation and convergence properties. Practical Lanczos procedures. Applications to $A x=b$ and least squares. Arnoldi and unsymmetric Lanczos.
10. Iterative Methods for Linear Systems. Standard iterations. Conjugate gradient method. Preconditioned conjugate gradients. Other Krylov subspace methods.
11. Functions of Matrices. Eigenvalue methods. Approximation methods. The matrix exponential.
12. Special Topics. Constrained least squares. Subset selection using SVD. Total least squares. Computing subspaces using SVD. Updating matrix factorizations. Modified/structured eigenproblems.

## Suggested Texts and References

- Matrix Computations, Gene H. Golub and Charles F. van Loan, The Johns Hopkins University Press (Third Edition, 1996).
- An Introduction to the Conjugate Gradient Method Without the Agonizing Pain, Jonathan Richard Shewchuck, Carnegie Mellon School of Computer Science Techincal Report CS-94-125 (1994). Available as a public web resource at http://historical.ncstrl.org/tr/ps/cmucs/CMU-CS-94-125.ps.


## B.4.4 Miscellaneous Topics in Numerical Analysis

Number of Lectures - 5
Prerequisites • None

## Syllabus

1. Miscellaneous topics in numerical analysis. Topics of practical importance that are not covered in any of the rest of the modules.

## Suggested Texts and References

- Numerical Recipes in C: The Art of Scientific Computing, William H. Press, Brian P. Flannery, Saul A. Teukolsky, and William T. Vetterling, Cambridge University Press (second edition, 1992). Indian edition/reprint available. Available as a public web resource at http://lib-www.lanl.gov/numerical/.


## B. 5 Perspectives on Probability Modeling I (CMS-M\&S-1-5)

## B.5.1 Reasoning Under Uncertainty

Number of Lectures • 25
Prerequisites • B.1.3
Syllabus

1. Models, Statistical Inference and Learning. Parametric and nonparametric models. Fundamental concepts in inference: point estimation, confidence sets, hypothesis testing.
2. Estimating the CDF and Statistical Functionals. The empirical distribution function. Statistical functionals.
3. The Bootstrap. Introduction. Simulation strategy. Bootstrap variance estimation. Bootstrap confidence intervals. Jackknife. Justification for the percentile interval.
4. Parametric Inference. Parameter of interest. The method of moments. Maximum likelihood. Properties of maximum likelihood estimators. Consistency of maximum likelihood estimators. Equivariance of the MLE. Asymptotic normality. Optimality. The delta method. Multiparameter models. The parametric bootstrap. Checking assumptions. Computing maximum likelihood estimates and the EM algoithm.
5. Hypothesis Testing and $p$-Values. The Wald test. $p$-values. The $\chi^{2}$ distribution. Pearson's $\chi^{2}$ test for multinomial data. The permutation test. The likelihood ratio test. Multiple testing. Goodness-of-fit tests. The Neyman-Pearson lemma. The $t$-test.
6. Bayesian Inference. The Bayesian philosophy. The Bayesian method. Functions of parameters. Simulation. Large sample properties of Bayes procedures. Flat priors, improper priors and "noninformative" priors. Multiparameter problems. Bayesian testing. Strengths and weaknesses of Bayesian inference.
7. Statistical Decision Theory. Comparing risk functions. Bayes estimators. Minimax rules. Maximum likelihood, minimax and Bayes. Admissibility. Stein's paradox.

## Suggested Texts and References

- All of Statistics, Larry Wasserman, Springer-Verlag (2004).
- Mathematical Statistics, John E. Freund, Prentice-Hall of India (fifth Indian reprint, 1998). Indian edition/reprint available.
- Probability and Statistics, Morris deGroot and Mark Schervish, Addison-Wesley (third edition, 2002).


## B.5.2 Stochastic Simulation

Number of Lectures • 15
Prerequisites • B.1.3

## Syllabus

1. Introduction: Integration by Simulation. Error propagation in numeric versus stochastic integration methods. Exact sampling methods. Importance sampling.
2. A Tutorial on "Random" Numbers. Uniform distribution and linear congruential generators. Correlations and the Marsaglia lattice structure. Randomness and complexity. Tests for randomness. Exponential distribution and the transformation method. Box-Muller method. Other distributions. Arbitrary distributions and the rejection method.
3. Integration by Simulation: The Rejection Method. Best $g$ is $f$ itself. The acceptance complement method. A trivial perfect MCMC method.
4. A Statistical Physics Perspective on MCMC. From Newton to Hamilton. Hamiltonian Formulation. Phase Space. Maxwell-Boltzmann-Gibbs Distribution. The Original Metropolis Algorithm Circa 1953. Simulated Annealing Circa 1983.
5. Connection with Statistics. Probabilistic inference with a fully-specified model. Statistical inference for model parameters. Bayesian inference, model comparison and model averaging. Statistical physics.
6. The Monte Carlo Problem and its Solution. Definition of the problem. Approaches to solving the problem. Theory of Markov chains.
7. The Metropolis and Gibbs Sampling Algorithms. Gibbs sampling. The Metropolis algorithm. Variations on the Metropolis algorithm. Analysis of the Metropolis and Gibbs sampling algorithms.
8. Extensions and Refinements. Dynamical and hybrid Monte Carlo Methods, stochastic dynamics methods, a hybrid Monte Carlo algorithm with analysis, other dynamical methods. Simulated annealing. Free energy estimation. Error assessment and reduction. Parallel implementation.

## Suggested Texts and References

- Probabilistic Inference Using Markov Chain Monte Carlo Methods, Radford M. Neal, Technical Report CRG-TR-93-1, Department of Computer Science, University of Toronto. Available as a public web resource at http://www.cs.toronto.edu/~radford/review.abstract.html


## B.5.3 Stochastic Differential Equations

Number of Lectures • 5
Prerequisites • None
Syllabus Introduction to stochastic differential equations and its applications.
Suggested Texts and References
B. Oksendal, Stochastic Differential Equations, An introduction with Applications (Springer, 1998).

## B. 6 Perspectives on Probability Modeling II (CMS-M\&S-2-6)

## B.6.1 Statistical Models and Methods

Number of Lectures • 25
Prerequisites • B.5.1
Syllabus

1. Linear and Logistic Regression. Simple Linear Regression. Least Squares and Maximum Likelihood. Properties of the Least Squares Estimators. Prediction. Multiple Regression. Model Selection. Logistic Regression.
2. Multivariate Models. Random vectors. Estimating the correlation. Multivariate normal. Multinomial.
3. Inference about Independence. Two binary variables. Two discrete variables. Two continuous variables. One continuous variable and one discrete variables.
4. Causal Inference. The counterfactual model. Beyond binary treatments. Observational studies and confounding. Simpson's paradox.
5. Directed Graphs and Conditional Independence. Conditional independence. Directed graphs. Probability and directed graphs. More independence relations. Estimation for directed graphs.
6. Undirected Graphs. Undirected graphs. Probability and graphs. Cliques and potentials. Fitting graphs to data.
7. Log-Linear Models. The log-linear model. Graphical log-linear models. Hierarchical log-linear models. Model generators. Fitting log-linear models to data.
8. Nonparametric Curve Estimation. The bias-variance tradeoff. Histograms. Kernel density estimation. Nonparametric regression.
9. Smoothing Using Orthogonal Functions. Orthogonal functions and $L_{2}$ spaces. Density estimation. Regression. Wavelets.
10. Classification. Error rates and the Bayes classifier. Gaussian and linear classifiers. Linear regression and logistic regression. Relationship between logistic regression and linear discrimination analysis. Density estimation and naive Bayes. Trees. Assessing error rates and choosing a good classifier. Support vector machines. Kernelization. Other classifiers.
11. Time Series Analysis. Overview of the Box-Jenkins and Bayesian approaches. Principles of nonlinear and chaotic time series analysis.

## Suggested Texts and References

- All of Statistics, Larry Wasserman, Springer-Verlag (2004).
- Mathematical Statistics, John E. Freund, Prentice-Hall of India (fifth Indian reprint, 1998). Indian edition/reprint available.
- Probability and Statistics, Morris deGroot and Mark Schervish, Addison-Wesley (third edition, 2002).
- Time Series Analysis: Forcasting and Control, G. E. Box, G. M. Jenkins and G. Reinsel, Prentice-Hall (3rd edition, 1994). ISBN 0130607746.
- Nonlinear Time Series Analysis, H. Kantz and T. Schreiber, Cambridge University Press (2nd edition, 2004). ISBN 0521529026.


## B.6.2 Stochastic Optimization

Number of Lectures • 20
Prerequisites - B.5.2

## Syllabus

1. Stochastic Search and Optimization. Principles, motivation and supporting results. Direct methods for stochastic search: random search with noise-free loss measurements, random search with noisy loss measurements, nonlinear simplex (Nelder-Mead) algorithm.
2. Stochastic Approximation for Nonlinear Root-Finding. Examples. Convergence of stochastic approximation. Asymptotic normality and choice of gain sequence. Extensions to basic stochastic approximation.
3. Stochastic Gradient Form of Stochastic Approximation. Root-finding stochastic approximation as a stochastic gradient method. Neural network training. Discrete-event dynamic systems. Image restoration.
4. Stochastic Approximation and the Finite-Difference Method. Some motivating examples for gradient-free stochastic approximation. Finite-difference algorithm. Convergence theory. Asymptotic normality. Practical selection of gain sequences. Several finite-difference examples. Some extensions and enhancements to the finite-difference algorithm.
5. Annealing-Type Algorithms. Simulated annealing algorithm. Examples. Global optimization via annealing algorithms based on stochastic approximation. Convergence theory for simulated annealing based on stochastic approximation.
6. Evolutionary Computation I: Genetic Algorithms. Historical perspective and motivating applications. Coding of elements for searching. Standard genetic algorithm operations. Overview of basic GA search approach. Practical guidance and extensions: coefficient values, constraints, noisy fitness evaluations, local search, and parent selection. Examples.
7. Evolutionary Computation II: General Methods and Theory. Overview of evolution strategy and evolutionary programming with comparisons to genetic algorithms. Schema theory. What makes a problem hard? Convergence theory. No free lunch theorems.
8. Evolutionary Computation III: Particle Swarm Optimization.
9. Statistical Methods for Optimization in Discrete Problems. Statistical comparisons test without prior information. Multiple comparisons against one candidate: with known noise variance(s), with unknown noise variance(s). Extensions to Bonferroni inequality; ranking and selection methods in optimization over a finite set.
10. Simulation-Based Optimization I: Regeneration, Common Random Numbers, and Selection Methods. Background. Regenerative systems. Optimization with finite-difference and simultaneous perturbation gradient estimators. Common random numbers. Selection methods for optimization with discrete-valued $\theta$.
11. Simulation-Based Optimization II: Stochastic Gradient and Sample Path Methods. Framework for gradient estimation. Pure likelihood ratio/score function and pure infinitesimal perturbation analysis. Gradient estimation methods in rootfinding stochastic approximation: the hybrid LR/SF and IPA setting. Sample path optimization.
12. Introduction to Optimization Under Uncertainty. Optimization problems where some of the constrains include random (stochastic) components, such as online optimization under time constraints, stochastic load balancing and related problems, stochastic knapsack problem, stochastic combinatorial and discrete optimization problems, stochastic approaches to supply chain management problems.

## Suggested Texts and References

- Introduction to Stochastic Search and Optimization: Estimation, Simulation, and Control, J. C. Spall, John Wiley and Sons, Inc. (2003). ISBN 0471330523. Associated website: http://www.jhuapl.edu/ISSO/.
- Simulated Annealing: Theory and Applications, P. J. M. Van Laarhoven and E. H. L. Aarts, Kluwer Academic Publishers (1987). ISBN 9027725136.
- Optimization by Simulated Annealing, S. Kirkpatrick, C. D. Gelatt Jr, and M. P. Vecchi, Science 220, 671680 (1983).
- Stochastic Programming Bibliography, Maarten H. van der Vlerk (1996-2003). Available as a public web resource at http://mally.eco.rug.nl/spbib.html.
- Swarm intelligence and optimization resources: http://clerc.maurice.free.fr/pso/, http://www.swarmintelligence.org/, http://dsp.jpl.nasa.gov/members/payman/swarm/.


## B. 7 Practical Computing I (CMS-M\&S-1-7)

## B.7.1 Truncated Numbers and Finite-Precision Arithmetic

Number of Lectures • 3
Prerequisites • None

## Syllabus

1. Computer Representation of Numbers. Introduction, principles and issues. Representation of integers and properties of the representation. Overflow. Endianness.
2. Representation of Real Numbers. Rational numbers. Fixed-point and floatingpoint representations. Properties of floating-point numbers. Number and distribution of representable floating-point numbers. Overflow and underflow.
3. Finite-Precision Arithmetic with Floating-Point Numbers. How elementary arithmetic operations are performed. Subtraction and loss of precision. Illustrative examples.
4. A User's Perspective on IEEE 754. The IEEE 754 specification. All about NaNs and Infs. Tracking floating-point exceptions. Outlook on IEEE 754.

## Suggested Texts and References

- What Every Computer Scientist Should Know About Floating-Point Numbers, David Goldberg, Computing Surveys (March, 1991). Available as a public web resource at http://docs.sun.com/source/806-3568/ncg_goldberg.html.
- The Art of Computing, vol. II: Seminumerical Algorithms, Donald E. Knuth, Addison-Wesley (third edition, 1997).
- Numerical Recipes in C: The Art of Scientific Computing, William H. Press, Brian P. Flannery, Saul A. Teukolsky, and William T. Vetterling, Cambridge University Press (second edition, 1992). Indian edition/reprint available. Available as a public web resource at http://lib-www.lanl.gov/numerical/.

Module contributed by Mihir Arjunwadkar

## B.7.2 Systems Modeling and Simulation

Number of Lectures • 15
Prerequisites • None
Syllabus

1. Describing Systems. The Nature of Systems. Event Driven Models. Characterizing Systems. Simulation Diagrams. The System Aproach.
2. Dynamical system. Initial Value problem. Higher Order syetms. Autonomous Dynamic Systems. Multiple time based systems. Handling Empirical Data.
3. Modeling. Stochastic Generators. Spatial Distributions. Stochastic Data Representation. Modeling Time-Driven Systems. Exogenous Signals and Events. Event-Driven Models. System Optimization.

## Suggested Texts and References

- System Modeling and Simulation: An Introduction, Frank L. Severance, John Wiley and Sons, Inc. (2001).
- Theory of Modeling and Simulation, Bernard Zeigler, Herbert Praehofer and T. G. Kim, Academic Press (1999). ISBN 0127784551.


## B.7.3 Programming Paradigms and Perspectives Hands-On

Number of Lectures • 10
Prerequisites • None
Syllabus

1. Types and variables Representation of primitive types, arrays, disjoint unions, recursive types etc. Storage for global and local variables, heap variables Implementation of static and dynamic arrays
2. Abstraction Implementation of procedure calls, method calls Objetcs, Parameter Passing, Generic Units, Critical regions
3. Type Systems and Control Flow Implementation of polymorphic procedures Implementation of jumps and escapes, exceptions
4. Paradigms Case studies taking specific language examples for Imperative Programming Object-Oriented Programming Concurrent Programming Functional Programming Logic Programming Scripting

## Suggested Texts and References

- See Texts and References for the Programming: Theory and Perspectives module, Section B.2.2.
B SYLLABUS


## B.7.4 Case Studies I

Number of Lectures • 17
Prerequisites • None
Syllabus

1. Hands-On Case Studies relevant to the Perspectives on Mathematical Modeling I (Section B.3) and Perspectives on Probability Modeling I (Section B.5) courses.

## Suggested Texts and References

## B. 8 Practical Computing II (CMS-M\&S-2-8)

## B.8.1 High-Performance Computing

Number of Lectures • 20
Prerequisites • None
Syllabus

1. Performance issues and measurement Profiling and development tools Sustained versus peak performance
2. High performance sequential computing Effects of the memory hierarchy Out-of-order execution superscalar processors
3. Vector processing
4. Shared-memory processing Architectures (extensions of the memory hierarchy), Programming paradigms, OpenMP
5. Distributed-memory processing Architectural issues (networks and interconnects), Programming paradigms, MPI (+MPI2)
6. Grids Computational grids, Data grids
7. Performance libraries and packages

## Suggested Texts and References

- High Performance Computing, 2nd Edition Charles Severance, Kevin Dowd O Reilly (2nd Edition July 1998 )
- MPI: The Complete Reference (Vol. 2 - The MPI-2 Extensions) Marc Snir, Steve Otto, Steven Huss-Lederman, David Walker, and Jack Dongarra MIT Press (1998)


## B.8.2 Case Studies II

Number of Lectures • 25
Prerequisites • None
Syllabus

1. Hands-On Case Studies relevant to the Perspectives on Mathematical Modeling II (Section B.4) and Perspectives on Probability Modeling II (Section B.6) courses.

Suggested Texts and References

## B. 9 Elective (CMS-M\&S-2-9)

Number of Credits - 4
Syllabus for the Electives will be developed as and when required, depending on the electives offered during a programme year; see Section 7.3.
B. 10 Project (CMS-M\&S-3-10)

Number of Credits • 12
See Section 7.4.
B. 11 Term Papers (CMS-M\&S-3-11)

Number of Credits - 4
See Section 7.5.


[^0]:    ${ }^{1}$ In future, the $M \& S$ programme may also be run in a part-time mode ( 7.5 contact hours per week + minimum programme duration of 24 months). The Centre does not plan to run the M\&S programme in the part-time mode during academic year 2005-06 or in the near future.

[^1]:    ${ }^{2}$ This last alternative is most suitable for an institution like the Department of Computer Science, where the focus is quite different, and simulation is one part of the many aspects that need to be covered. We disregard this alternative for the M\&S Programme.
    ${ }^{3}$ Needless to say that the Centre plans not to do so before the M\&S Programme and the Centre itself are well-established.

[^2]:    ${ }^{4}$ Note that it may not be possible to offer the same set of electives every year. Whether a particular elective could be offered during a specific programme year depends on the availability of a domain expert in the respective domain.

