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COURSE OUTLINE

MATH5805

ADVANCED MONTE CARLO METHODS

Semester 2, 2016

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MATH5805 – Course Outline

1 Information about the course

Course Name: Advanced Monte Carlo Methods
Course Authority and Lecturer: Pr. Pierre Del Moral, email: p.del-moral@unsw.edu.au
Consultation: To be arranged via email.
UOC: 6
Prerequisites & Exclusions:

The course has been designed so that there are no fixed prerequisites. In particular, students do not need to have taken MATH5835 (Stochastic Processes). However, it will be assumed that participants will have a good knowledge of probability theory and basic Markov chain models. In particular, a good knowledge of undergraduate mathematics and of undergraduate probability at the level of MATH2801/MATH2901 is required. This means familiarity with basic probability models, random variables and their probability distributions, independence, expectations and conditional probabilities, as well as the law of large numbers. If you need a thorough review of basics, the textbook Probability by Jim Pitman is recommended.
Exposure to classical differential calculus, and basic vector and matrix algebra will be assumed also. Handouts or references to what is required by way of preparation will be available from the lecturer in the beginning of August upon request.
Lectures: 17:00–20:00 on Mondays and Wednesdays, in the Red Centre Central Wing Room 1040 (starting 1st August).

Moodle: Further information and skeleton lecture notes, and other materials will be provided via Moodle. Please check the course homepage regularly for updates.

2 Course outline

This course will cover topics in the general area of Monte Carlo methods and their application domains. The topics include Markov chain Monte Carlo and Sequential Monte Carlo methods, Quantum and Diffusion Monte Carlo techniques, as well as branching and interacting particle methodologies. The lectures cover discrete and continuous time stochastic models, starting from traditional sampling techniques (perfect simulation, Metropolis-Hasting, and Gibbs-Glauber models) to more refined methodologies such as gradient flows diffusions on constraint state space and Riemannian manifolds, ending with the more recent and rapidly developing Branching and mean field type Interacting Particle Systems techniques.

The course offers a pedagogical introduction to the theoretical foundations of these advanced stochastic models, combined with a series of concrete illustrations taken from different applica-tion domains. The applications considered in these lectures will range from Bayesian statistical learning (hidden Markov chain, statistical machine learning), risk analysis and rare event sam-pling (mathematical finance, and industrial risk assessment), operation research (global optimization, combinatorial counting and ranking), advanced signal processing (stochastic nonlinear filtering and control, and data association and multiple objects tracking), computational and statistical physics (molecular dynamics, Schrödinger's ground states, Boltzmann-Gibbs distributions, and free energy computation). Approximately the first half of the course will be concerned with linear type Markov chain Monte Carlo methods, and the second part to nonlinear particle type methodologies. A list of topics intended to be covered is attached.

Relation to other courses and relevant programs
This is an elective in the Master of Statistics, the Master of Biostatistics and the Master of Financial Mathematics.

3 Student Learning Outcomes

By the end of this course you will

1. Be familiar with the major types of advanced Monte Carlo models in discrete and continuous time.
2. Understand the mathematical foundations and the convergence properties of linear and nonlinear particle Markov chain algorithms.
3. Understand computational methodologies for sampling complex probability measures including conditional distributions (with respect to partial observation models and rare events) and more general Feynman-Kac distributions on path spaces.
4. Know about areas of applications of advanced Monte Carlo methods to statistical machine learning, risk and rare event analysis, mathematical finance, computational physics, etc.

Relation to graduate attributes
The above outcomes are related to the development of the Science Faculty Graduate Attributes, in particular (level of focus 1 =min, 2=minor, and 3 =major):

- **Research, inquiry and analytical thinking abilities (3)**: This attribute is central to the course, and will be developed in lectures, computer work, self-study, homework. All assessment tasks will assess your application of these skills.
- **Capability and motivation for intellectual development (3)**: Capacity to understand advanced theoretical and computational methods for complex distribution sampling and high dimensional integration.
- **Teamwork, collaborative and management skills (2)**: A teamwork research project will require collaborative research on an application domain selected by the student among the ones discussed in the course.

4 Teaching strategies underpinning the course

New ideas and skills are first introduced and demonstrated in lectures, then students develop these skills by applying them to specific tasks in assessments.

Rationale for learning and teaching strategies
We believe that effective learning is best supported by a climate of inquiry, in which students are actively engaged in the learning process. To ensure effective learning, students should participate in all lectures.

We believe that effective learning is achieved when students attend all classes, have prepared for classes by reading through previous lecture notes.

Furthermore, lectures should be viewed by the students as an opportunity to learn, rather than just to copy down lecture notes.

Effective learning is achieved when students have a genuine interest in the subject and make a serious effort to master the material.

The art of logically setting out mathematics is best learned by watching an expert and paying particular attention to detail. This skill can be learned by regularly attending classes.

5 Assessment

Assessment in this course will consist of 2 assignments ($2 \times 10\%$), a research project on a selected application domain (20%), and a final examination (60%).

Knowledge and abilities assessed: All assessment tasks will assess the learning outcomes outlined above, specifically, the ability to provide logical and coherent proofs of results and specific problems related to Monte Carlo methods.

Assessment criteria: The main criteria for marking all assessment tasks will be clear and logical presentation of correct solutions.

5.1 Assignments

Rationale Assignments will give an opportunity for students to try their hand at more difficult problems which require more than one line of argument and also induce them to aspects of the subject which are not always explicitly covered in lectures.

Assignment one will be handed out in the second lecture of week 2 and will be collected in the second lecture of week 3. Assignment two will be handed out in the first lecture of week 4 and will be collected the first lecture of week 6.

Assignments must be handed in by the due date and time. Late submission will not be accepted unless there is documentary evidence of mitigating circumstances.

Each assignment must include a signed declaration of the plagiarism coversheet which can be found on Moodle.

All work submitted for assessment (other than formal examination scripts) will be returned with comments where appropriate.

Assignments must be YOUR OWN WORK, or severe penalties will be incurred. Please refer to Section 9 for information on plagiarism.

Weighting: Each assignment weights 10% of your final mark. Students who miss an assigment will receive 0 marks unless they request special consideration in accordance with university guidelines. See
http://www.maths.unsw.edu.au/currentstudents/special-consideration-illness-misadventure

5.2 Research project

Rationale

Research projects offer the opportunity for students to apply the theory of stochastic processes to an application domain they will select among the ones discussed in the course:

Bayesian statistical learning (hidden Markov chain, statistical machine learning), risk analysis and rare event sampling (mathematical finance, and industrial risk assessment), operation research (global optimisation, combinatorial counting and ranking), advanced signal processing (stochastic nonlinear filtering and control, and multiple objects tracking), computational and statistical physics (molecular dynamics, quasi-invariant measures, particle absorption models, Schrödinger's ground states, Boltzmann-Gibbs distributions, and free energy computation), and many others.

The research project provides an opportunity to immerse the student in one of her/his favorite application area. To favor creativity, critical thinking, brainstorming, collaboration and organization, a given research project can be shared by two students.

Some material will be given to the students, but the research project also requires to do a background study and a personal research. The final research project will be written in the format of a pedagogical report with 10 to 20 pages. It will include the following sections: introduction, a section on the theoretical aspects and another on the numerical aspects (including if possible some simulation codes), and a final conclusion.

Weighting: 20% of your final mark.

Research project must be delivered in week 6. Late submission will not be accepted unless there is documentary evidence of mitigating circumstances.

Each research project must include a signed declaration of the plagiarism coversheet which can be found on Moodle.

All work submitted for research projects will be returned with detailed comments.

Nevertheless each project must be YOUR OWN WORK, or severe penalties will be incurred. Please refer to Section 9 for information on plagiarism.

5.3 Examination

Duration: Two hours.

Rationale: The final examination will assess student mastery of the material covered in the lectures. It also allows students to individually demonstrate their achievement of the course outcomes under controlled conditions independent of assistance from others.

Students who miss an exam will receive 0 marks unless they request special consideration in accordance with university guidelines. See
http://www.maths.unsw.edu.au/currentstudents/special-consideration-illness-misadventure

Weighting: 60% of your final mark.

Further details about the final examination will be made available in class closer to the time and also on WebCT.

5.4 Additional resources and support

5.4.1 Lecture notes

A set of lecture notes will be provided on Moodle. Some of them will contain the full presentation of a topic and it will be sufficient to learn the required material. Others will be more brief and contain a list of the results that should be studied using recommended textbooks.

5.4.2 Textbooks

The content of the course will be defined by the lectures. Self contained and detailed lecture notes for the course will be provided. Other textbooks which can be useful for supplemental reading are:

- Mean field simulation for Monte Carlo integration. P. Del Moral. Chapman & Hall/CRC Monographs on Statistics & Applied Probability (2013).
- Feynman-Kac formulae. Genealogical and interacting particle approximations. P. Del Moral. Springer New York. Series: Probability and Applications (2004).
- Free energy computation: a mathematical perspective. T. Lelièvre, M. Rousset and G. Stoltz. Imperial College Press (2010).
- A pedagogical introduction to quantum Monte Carlo. M. Caffarel, R. Assaraf in Mathematical models and methods for ab initio Quantum Chemistry in Lecture Notes in Chemistry, eds. M. Defranceschi and C.Le Bris, Springer p.45 (2000).
- Stochastic methods in quantum mechanics M. Caffarel in Numerical Determination of the Electronic Structure of Atoms, Diatomic and Polyatomic Molecules. Kluwer Academic Publishers (1989)

- Fundamentals of Stochastic Filtering. A. Bain and D. Crisan. Springer, Stochastic Modelling and Applied Probability, Vol. 60 (2009).
- Inference in Hidden Markov Models. O. Cappé, E. Moulines, and T. Ryden. Springer series in Statistics (2005).

6 Course Schedule

The topics will be selected from the following:

PART 1: Linear Monte Carlo methods

- Markov chains: martingale decompositions, invariant measures, stability properties, ergodic theorem, Monte Carlo simulation.
- Continuous time models: evolution semigroups, stability properties, illustrations, Monte Carlo simulation.
- Markov chain Monte Carlo models: Boltzmann-Gibbs target measures, Metropolis-Hasting model, Gibbs-Glauber dynamics, Propp and Wilson sampler, multilevel annealing models (simulated annealing, sequential multilevel algorithms).
- Advanced Markov chain monte Carlo models: continuous time embeddings, gradient flow models, diffusions on Riemannian manifolds, Metropolis-adjusted Langevin models.

PART 2: Illustrations

- Computational physics: Molecular dynamics, Hamiltonian and Langevin equations, Ising model, graph coloring problems, subset sampling.
- Bayesian inference: disintegration models, Gibbs sampling, conjugate priors, exponential family of distributions.
- Signal processing: Kalman filters, Backward smoothing, hidden Markov chains problems.

PART 3: Nonlinear Monte Carlo methods

- Nonlinear Markov chains models and their mean field particle interpretations.
- Branching and interacting particle interpretations of Feynman-Kac models: forward and backward particle models, particle normalizing constants, genealogical tree based algorithms.
- Particle Markov chain Monte Carlo methodologies: acceptance-rejection sampling with recycling, interacting Metropolis-Hasting model, Particle Gibbs-Glauber dynamics, interacting simulated annealing models, multi-splitting sampling techniques.

- Analysis toolbox: variance and bias expansions, stochastic perturbation analysis, backward semigroup expansions, exponential concentration inequalities.

PART 4: Illustrations

- Bayesian statistical inference: Particle Approximate Bayesian Computation methods, particle expectation maximisation algorithms, particle stochastic gradient models, particle Markov chain Monte Carlo methods for the estimation of fixed parameters in hidden Markov chains models.
- Signal processing: Ensemble Kalman filters and data assimilation problems, forward and backward particle filters, interacting Kalman filters, particle data association methodologies for solving multiple targets tracking problems.
- Computational physics: McKean Vlasov and Burgers models, particle approximation of quasi-invariant measures, free energy computation, particle absorption models in hard and soft obstacles, computation of the top of the spectrum and the ground state energies of Schrödinger operators, quantum and diffusion Monte Carlo methodologies.
- Operation research: risk analysis and rare event simulation: multi-level splitting techniques, particle subset sampling, black box and inverse problems.
- Mathematical finance: European and American option pricing, default probabilities, particle gradient estimates and Malliavin Greeks derivatives.

7 Course Evaluation and Development

The School of Mathematics and Statistics evaluates each course each time it is run. We carefully consider the student responses and their implications for course development. It is common practice to discuss informally with students how the course and their mastery of it are progressing.

8 Administrative matters

Expectations of Students, assessment policies	Important information for students (including rules and expectations for attendance, release of marks, additional assessment) is available from http://www.maths.unsw.edu.au/currentstudents/assessment-policies
Occupational Health and Safety	See http://www.gs.unsw.edu.au/policy/documents/ohspolicy.pdf for UNSW Occupational Health and Safety policies and expectations of students regarding health and safety.
Equity and Diversity	Those students who have a disability that requires some adjustment in their teaching or learning environment are encouraged to discuss their study needs with the course Convenor prior to, or at the commencement of, their course, or with the Equity Officer (Disability) in the Equity and Diversity Unit (9385 4734 or http://www.studentequity.unsw.edu.au/). Issues to be discussed may include access to materials, signers or note-takers, the provision of services and additional exam and assessment arrangements. Early notification is essential to enable any necessary adjustments to be made.
Grievance Policy	First, see your course authority! If resolution is not possible, then follow the procedures listed on the page https://my.unsw.edu.au/student/atoz/Complaints.html

9 Plagiarism and academic honesty

Plagiarism is the presentation of the thoughts or work of another as one's own. Issues you must be aware of regarding plagiarism and the university's policies on academic honesty and plagiarism can be found at http://www.lc.unsw.edu.au/plagiarism/.