Skoltech

Course Syllabus

Course Title	Stochastic Methods in Mathematical Modelling and Artificial Intelligence
Course Title (in Russian)	Стохастические методы в математическом моделировании и искусственном интеллекте
Lead Instructor	Palyulin, Vladimir

1. Annotation

Course Description

Stochastic processes play an important role in natural sciences, computational theory as well as in sampling and synthetic data generation for machine learning. The course aims to cover basic methods of stochastic modelling as well as the application towards generative models. These include Monte-Carlo methods, the modelling of scale-free phenomena as well as stochastic optimisation approaches.

The first part of the course provides an introduction to the methods of description and generation of randomness. The main idea is to establish a firm ground for more advanced topics and to help students feel comfortable with advanced machine learning courses. A special emphasis is put on the ubiquitous scale-free and non-gaussian stochastic processes also known as anomalous diffusion. Different causes of these processes will be discussed with examples such as practically important class of first-passage problems.

The second half of the course will deal with Monte-Carlo algorithms, diffusion generative models, inference and learning, classical random network theory, Markov decision processes and stochastic optimal control.

Course Description (in Russian)

Случайные процессы играют важную роль в различных областях естественных наук, вычислениях, а также для выборки и генерации синтетических данных в машинном обучении. Основной целью курса является обзор основных методов стохастического моделирования и их приложений к генеративному ИИ, включая методы Монте-Карло, моделирование процессов без характерного масштаба и методы стохастической оптимизации.
Первая часть курса посвящена методам генерации и описанию различных типов случайных процессов с целью обеспечить надежную базу для последующей части курса и курсов по машинному обучению. Особое внимание уделяется стохастическим дифференциальным уравнениям и основным моделям, описывающим негауссовскую статистику и процессы без характерного масштаба (аномальная диффузия).
Вторая часть курса посвящена методам Монте-Карло, классической теории сетей, диффузионным генеративным моделям, Марковским процессам принятия решений и стохастическому оптимальному контролю.

2. Basic Information

Course Academic Level	MSc, PhD
Number of ECTS credits	6

Course Prerequisites / Recommendations
calculus, ODEs, PDEs, probability theory

Type of Assessment	Graded

Mapping from grades to percentage:

A:	86
B:	76
C:	66
D:	56
E:	46
F:	0
Term	Term 2

Students of Which Programs do You Recommend to Consider this Course as an Elective?

BSc Programs	Masters Programs	PhD Programs
	Advanced Computational Science Data Science Internet of Things and Wireless Technologies	Computational and Data Science and Engineering Physics

Maximum Number of Students

	Maximum Number of Students
Overall:	30
Per Group (for seminars and labs):	30

3. Course Content

Topic	Summary of Topic	Contact Hours: Lectures	Contact Hours: Seminars	Contact Hours: Labs	Non-contact Hours: Student's Independent Study
Random variables	Characterisation and description. Operations & Transformations. Moments/Averages/Cumulants/Generation Function in Examples. Example of Gaussian Variables: Matrix Inversion, Normalization, Moments. Correlations and copulas	3	3	1	16
Distributions	Distribution sampling. Inverse transform sampling. Box-Muller. Extreme value statistics	3	6	2	17
Stochastic differential equations	Langevin and Fokker-Planck approaches for stochastic problems. Examples of SDEs with solutions. First-passage paradigm. Applications of first-passage theory.	3	3	1	20
Diffusion models and the optimal transport	Diffusion models. Rectified flows. Optimal transport	3	3	1	10
Non-Gaussian and scale-free randomness. Anomalous diffusion	Anomalous stochastic processes. CTRW with derivation. Fractional Fokker-Planck equations. Introduction into fractional calculus. Ageing. Fractional Brownian Motion. Sinai diffusion. First arrival, most reliable search.	3	3	1	10
Monte-Carlo algorithms	Markov chains. Monte-Carlo Algorithms: General Concepts and Direct Sampling. Markov-Chain Monte-Carlo. MC convergence.	3	6	1	16

Topic	Summary of Topic	Contact Hours: Lectures	Contact Hours: Seminars	Contact Hours: Labs	Non-contact Hours: Student's Independent Study
Modelling and optimisation	Queuing Systems. Markov Decision Processes & Stochastic Optimal Control	3	6	1	14

4. Learning Outcomes

Skoltech Learning Outcomes are indicated as per Skoltech Learning Outcomes Framework.

1. FUNDAMENTAL KNOWLEDGE

1.1. KNOWLEDGE OF MATHEMATICS AND NATURAL SCIENCES

2.1. COGNITION AND MODES OF REASONING

2.1.1. Analytical reasoning and problem solving

2.1.2. System thinking

2.2. ATTITUDES AND LEARNING PROCESS

2.2.1. Initiative and the willingness to take appropriate risks

2.2.3. Responsibility, intensity, perseverance, urgency and will to deliver

2.2.5. Self-awareness and a commitment to self-improvement, lifelong learning and educating

3.1. COMMUNICATIONS IN INTERNATIONAL ENVIRONMENTS

3.1.2. Written, electronic and graphical communication

3.1.3. Oral presentation and discussion

3.1.5. Communications in English in scientific, business and social settings

5. Assignments and Grading

Physical Attendance Requirement (% of classes)	80

Assignment Type	Assignment Summary	% of Final Course Grade
Homework Assignments	Homework 1. 4 problems (analytical and numerical). Inverse Transform Sampling. Transformation of PDFs. Correlated random variables.	10
Homework Assignments	Homework 2. 4 problems (analytical and numerical). Markov Chains.	10

Assignment Type	Assignment Summary	% of Final Course Grade
Homework Assignments	Homework 3. 4 problems (analytical and numerical). Stochastic differential equations. Fokker-Planck equations.	10
Homework Assignments	Homework 4. 4 problems (analytical and numerical). Monte-Carlo simulations. Direct and MCMC.	10
Final Exam	4 analytically solvable problems covering the main topics of the course.	20
Final Project	Read and reproduce results from a selected recent paper in the field	40

6. Assessment Criteria

Assignment 1 Type

Homework Assignments

Sample of Assignment 1

Input Sample of Assignment 1
Dice game
Assume that you play a dice game 100 times. Awards for the game are as follows
1, 3 or 5: 0$
2 or 4: 2$
6: 26$
(i) Estimate expected value of winnings
(ii) Estimate standard deviation of winnings
(iii) Estimate probability of winning at least 200$
[hint: use central limit theorem]

Assessment Criteria for Assignment 1

Graded from 0 to 10 for the whole homework. The points are split between the exercises depending on the expected time for solving them.
100 percent points are given for the complete solution with a correct answer.
80 percent of points are awarded if there is an insignificant arithmetic type error, but all the steps are right.
40 percent points for an exercise are given if there are some steps which are right but the solution is not
Smaller percentage could be granted if there are some correct steps but generally the solution is wrong.
The number of points for the exercise is obtained by multiplication of the percentage described above on the whole value of the exercise.

Assignment 2 Type

Homework Assignments

Sample of Assignment 2

Queue with finite buffer

Jobs arrive at the single server queuing station according to an exponential (Poisson) distribution with the rate λ. The waiting room of the server has finite capacity, N . If the waiting room is full, newly arrived particle is rejected (leaves the system), otherwise the particle is placed in the queue. Server picks up the jobs for processing from the
queue one by one, according to the first-come-firsts-served protocol. Assuming that

the probability distribution of the service processing time is exponential (Poisson) with rate μ,
(i) Compute the steady-state probability distribution p(n) of observing n jobs in the queue. What is the condition for a steady-state existence?
Assuming additionally that the system is in the steady-state,
(ii) Compute the expected number of customers in the queue.
(iii) Compute probability of (job's) rejection.
(iv) For $\lambda = 15$ hour -1 , $\mu = 10$ hour -1 and $N = 10$, compute the expected number of customers which are served between 10 am and 11 am.

Graded from 0 to 10 for the whole homework. The points are split between the exercises depending on the expected time for solving them.
100 percent points are given for the complete solution with a correct answer.
80 percent of points are awarded if there is an insignificant arithmetic type error, but all the steps are right.
40 percent points for an exercise are given if there are some steps which are right but the solution is not
Smaller percentage could be granted if there are some correct steps but generally the solution is wrong.
The number of points for the exercise is obtained by multiplication of the percentage described above on the whole value of the exercise.

Assignment 3 Type | Final Project

Sample of Assignment 3

Read the paper "Universal Generation of Statistical Self-Similarity: A Randomized Central Limit Theorem" by I. Eliazar, and J. Klafter published in Phys Rev Lett, 103, 040602 (2009). Program and reproduce the plots from the paper. Write a report. Present the results in a short 12 min talk

Assessment Criteria for Assignment 3

Report contributes 75 per cent of the project grade. Presentation adds another 25 per cent.

Assignment 4 Type | Final Exam

Sample of Assignment 4

Diffusion in a circle (5 marks)
Particle moves around a circle, $\varphi \in [0, 2\pi]$, according to the following stochastic equation
$d\varphi/dt = \omega + \xi$, (1)
where ω is a constant velocity and ξ(t) is a random correction, modeled as the white noise, i.e. hξ(t)i = 0 and = 2Dδ(t1 − t2). Assuming that φ(t = 0) = 0,
(i) Calculate the evolution of the mean value .
(ii) Calculate a probability to discover particle in a state φ at the moment of time, t.

Assessment Criteria for Assignment 4

Graded from 0 to 20 for the whole exam. The points are split between the exercises depending on the expected time for solving them.
100 percent of marks are given for the complete solution with a correct answer.
80 percent of marks are awarded if there is an insignificant arithmetic type error, but all the steps are right.
40 percent of marks for an exercise are given if there are some steps which are right but the solution is not complete.
Smaller percentage could be granted if there are some correct steps but generally the solution is wrong.
The number of points for the exercise is obtained by multiplication of the percentage described above on the whole value of the exercise.

7. Textbooks and Internet Resources

You can request at most two required textbooks. Additionaly, you can suggest up to nine recommended textbooks.

Required Textbooks	ISBN-13 (or ISBN-10)
Van Kampen N. G. Stochastic Processes in Physics and Chemistry (North-Holland, Amsterdam, 2001)	9780444529657
C. W. Gardiner, Handbook of stochastic methods for physics, chemistry and the natural sciences, 3rd ed., ser. Springer Series in Synergetics. Berlin: Springer-Verlag, 2004, vol. 13.	9783540707127

Recommended Textbooks	ISBN-13 (or ISBN-10)
M. Mézard and A. Montanari, Information, Physics, and Computation, Oxford University Press, 1st ed., 2009	9780198570837
D. J. C. Mackay, Information theory, inference, and learning algorithms. Cambridge: Cambridge University Press, 2003.	9780521642989

8. Facilities

Software
python

9. Additional Notes

The proposed course 1) has explicit academic content and requirements for receiving credits, 2) is in alignment with the program's learning outcomes, 3) adheres to policies and Skoltech regulations.

Lead Instructor confirms