Course guide
230861 - SM - Stochastic Methods for Optimization and Simulation

Last modified: 14/12/2023

Unit in charge: Barcelona School of Telecommunications Engineering
Teaching unit: 748 - FIS - Department of Physics.

Degree: MASTER'S DEGREE IN ENGINEERING PHYSICS (Syllabus 2018). (Optional subject).
ERASMUS MUNDUS MASTER'S DEGREE IN BIO & PHARMACEUTICAL MATERIALS SCIENCE (Syllabus 2021). (Optional subject).

Academic year: 2023 **ECTS Credits:** 4.0 **Languages:** English

LECTURER

Coordinating lecturer: Consultar aquí / See here: https://telecos.upc.edu/ca/estudis/curs-actual/professorat-responsables-coordinadors/responsables-assignatura

Others: Consultar aquí / See here: https://telecos.upc.edu/ca/estudis/curs-actual/professorat-responsables-coordinadors/professorat-assignat-idioma

PRIOR SKILLS

Calculus (differential and integral). Basic experience in numerical computer programming.

REQUIREMENTS

No requirements

DEGREE COMPETENCES TO WHICH THE SUBJECT CONTRIBUTES

Basic:
CB7. Students should know how to apply the knowledge acquired and their problem-solving ability in new or little-known environments within broader (or multidisciplinary) contexts related to their area of ¿¿study.
CB8. Students should be able to integrate knowledge and face the complexity of formulating judgments based on information that, being incomplete or limited, includes reflections on the social and ethical responsibilities linked to the application of their knowledge and judgment.

TEACHING METHODOLOGY

-Master classes
-Class exhibitions
-Team work
-Written work
-Problem resolution
-Practical exercises

LEARNING OBJECTIVES OF THE SUBJECT

- Ability to generate random numbers according to simple probability distribution laws

- Ability to perform a multidimensional integral using the Monte Carlo method and correctly estimate its statistical variance

- Know the methods for reducing variance and their optimal choice according to the type of problem to be solved

- Know how to make a calculation program for the classical simulation of a multiparticulate system using the Metropolis method

- Ability to perform multidimensional optimization using stochastic techniques

- To know the main stochastic methods used in the study of quantum systems

STUDY LOAD

Type	Hours	Percentage
Self study	64,0	64.00
Hours large group	36,0	36.00

Total learning time: 100 h

CONTENTS

Stochastic methods for optimization and simulation

Description:
1. Monte Carlo integration: distribution functions and their sampling, crude Monte Carlo, rejection, variance reduction techniques, multidimensional integration, Metropolis method.

2. Monte Carlo optimization: simulated annealing, genetic algorithms. Optimal control theory

3. Application of Monte Carlo methods to many particles systems. Discrete and continuous systems. Classical simulation of condensed phase systems: simple monoatomic systems, molecular materials, bio-molecules.

4. Dynamic Monte Carlo: random paths and diffusion equation, Fokker-Planck and Langevin methods, Brownian dynamics.

5. Applications of Monte Carlo methods to quantum systems: wave functions for bosons and fermions, variational Monte Carlo, diffusive Monte Carlo, path integral Monte Carlo.

Specific objectives:
Knowledge of the techniques in optimal control theory and the ability to apply Monte Carlo methods to find the optimal solution.

Know how to make a classical simulation of a multiparticle system using the Metropolis method.

Understand the basic theory of quantum Monte Carlo, and to know how to build a Monte Carlo program for the calculation of its properties.

Related activities:
Lectures

Assisted practices

Development of Monte Carlo programs

Autonomous learning

Related competencies :
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Full-or-part-time: 100h
Theory classes: 24h
Practical classes: 10h
Guided activities: 10h
Self study : 56h

GRADING SYSTEM

Oral presentation 25%
Works carried out by the student 75%

No reassessments will be made.

EXAMINATION RULES.

Presentation of practical work in the classroom with computer equipment.

Evaluable written report.

BIBLIOGRAPHY

Basic:
- Duchi, John C. Introductory lectures on stochastic optimization [on line]. [Stanford]: Park City Mathematics Institute, Graduate Summer School Lectures [, 2016Available on: https://stanford.edu/~jduchi/PCMIConvex/.
- Kalos, Malvin H. Monte Carlo methods [on line]. Weinheim: Wiley-Blackwell, 2008 [Consultation: 18/06/2021]. Available on: https://onlinelibrary.wiley.com/doi/book/10.1002/9783527626212. ISBN 9783527407606.
- Frenkel, D.; Smit, B. Understanding molecular simulation: from algorithms to applications [on line]. London: Academic Press is an imprint of Elsevier, 2023 [Consultation: 28/09/2023]. Available on: https://sciencedirect.com/book/9780323902922. ISBN 9780323913188.

RESOURCES

Computer material:
- Programació científica. Scientific programming languages and visualization tools