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

Last modified: 03/06/2022

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: 2022 **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. (ENG) Que los estudiantes sepan aplicar los conocimientos adquiridos y su capacidad de resolución de problemas en entornos nuevos o poco conocidos dentro de contextos más amplios (o multidisciplinares) relacionados con su área de estudio.
CB8. (ENG) Que los estudiantes sean capaces de integrar conocimientos y enfrentarse a la complejidad de formular juicios a partir de una información que, siendo incompleta o limitada, incluya reflexiones sobre las responsabilidades sociales y éticas vinculadas a la aplicación de sus conocimientos y juicio.

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

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 :
CB8. (ENG) Que los estudiantes sean capaces de integrar conocimientos y enfrentarse a la complejidad de formular juicios a partir de una información que, siendo incompleta o limitada, incluya reflexiones sobre las responsabilidades sociales y éticas vinculadas a la aplicación de sus conocimientos y juicio.
CB7. (ENG) Que los estudiantes sepan aplicar los conocimientos adquiridos y su capacidad de resolución de problemas en entornos nuevos o poco conocidos dentro de contextos más amplios (o multidisciplinares) relacionados con su área de estudio.

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, Daan. Understanding molecular simulation : from algorithms to applications. San Dieho [etc.]: Academic Press, 2002. ISBN 0122673514.

RESOURCES

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