PX914-15 Predictive Modelling and Uncertainty Quantification

24/25

Department
Physics
Level
Taught Postgraduate Level
Module leader
James Kermode
Credit value
15
Module duration
11 weeks
Assessment
60% coursework, 40% exam
Study location
University of Warwick main campus, Coventry

Description

Introductory description

N/A.

Module web page

Module aims

To equip students with tools to quantify the uncertainties in the outputs of their computational simulations

Outline syllabus

This is an indicative module outline only to give an indication of the sort of topics that may be covered. Actual sessions held may differ.

Introduction to uncertainty, probability and statistics (L1-2)
Sensitivity analysis (L3)
Linear regression (L4)

Uncertainty propagation using Monte Carlo sampling (L6)
Surrogate models - Gaussian process regression (L5), Polynomial Chaos (L7)
Inverse problems (L8)
Guest lecture on advanced topics in predictive modelling (L9)

Learning outcomes

By the end of the module, students should be able to:

- Demonstrate knowledge of statistical and mathematical methods for predictive modelling.
- Perform detailed, advanced analyses of complex data sets, extracting information and developing relationships using linear and nonlinear regression and classification techniques.
- Systematically develop models for predictive purposes using advanced techniques of model selection and evaluation.
- Understand and apply cutting-edge methods of machine learning.
- Demonstrate an understanding of complex modelling transferability issues arising from, e.g. choices of exchange-correlation functionals and pseudo-potentials in electronic structure, or the choice of force fields in atomistic and molecular models.
- Demonstrate a detailed knowledge of, and be able to apply models, for quantifying uncertainties arising in material structure and properties, constitutive models, from limited data scenarios and through coarse graining.

Indicative reading list

The recommended textbook is:

McClarren, Uncertainty Quantification an Predictive Computational Science, available from SpringerLink on campus at Warwick - aimed at a general Physical Sciences / Engineering audience
For a more mathematical viewpoint, some students may be interested in:

Sullivan, Introduction to Uncertainty Quantification, available from SpringerLink on campus at Warwick
Familiarity with vectors, matrices and basic linear algebra at the level taught in most undergraduate physical sciences and engineering courses will be assumed. If you would like to refresh your knowledge on this topic you may find the following resources useful:

Boyd and Vandenberghe, Introduction to Applied Linear Algebra - Vectors, Matrices and Least Squares, freely available online. Companion exercises that implement the material in Python and Julia are available from the same webpage.
Where appropriate, specific lectures also point to additional textbooks for relevant topics.

Subject specific skills

Demonstrate knowledge of statistical and mathematical methods for predictive modelling
Perform detailed, advanced analyses of complex data sets, extracting information and developing relationships using linear and nonlinear regression and classification techniques
Systematically develop models for predictive purposes using advanced techniques of model

selection and evaluation
Understand and apply cutting-edge methods of machine learning
Demonstrate an understanding of complex modelling transferability issues arising from, e.g. choices of exchange-correlation functionals and pseudo-potentials in electronic structure, or the choice of force fields in atomistic and molecular models.
Demonstrate a detailed knowledge of, and be able to apply models, for quantifying uncertainties arising in material structure and properties, constitutive models, from limited data scenarios and through coarse graining.

Transferable skills

Mathematical analysis, statistics, coding, writing

Study

Teaching split

Provider	Weighting
School of Engineering	80%
Warwick Mathematics Institute	20%

Study time

Type	Required
Lectures	10 sessions of 2 hours (13%)
Practical classes	8 sessions of 3 hours (16%)
Private study	66 hours (44%)
Assessment	40 hours (27%)
Total	150 hours

Private study description

Consolidation of lecture materials.
Further reading to support workshop and oral examination.

Costs

No further costs have been identified for this module.

Assessment

You do not need to pass all assessment components to pass the module.

Assessment group D1

	Weighting	Study time	Eligible for self-certification
Assessment component			
Assessed work	60%	30 hours	No

1. Based on the machine learning workshop exercises.
2. Based on the uncertainty propagation workshop.
3. Based on predictive multiscale modelling.

Reassessment component is the same

Assessment component			
Viva voce Exam	40%	10 hours	No

On the core material. 30 minutes.

Reassessment component is the same

Feedback on assessment

Written annotations to submitted computational notebooks\r\n-\tVerbal discussion during viva voce exam\r\n-Written summary of viva performance

Past exam papers for PX914

Availability

Courses

This module is Core for:

- Year 1 of TPXA-F344 Postgraduate Taught Modelling of Heterogeneous Systems
- Year 1 of TPXA-F345 Postgraduate Taught Modelling of Heterogeneous Systems (PGDip)