TO: The Engineering Faculty

FROM: The Faculty of the School of Mechanical Engineering

RE: New Course - ME 53900 Introduction to Scientific Machine Learning

The Faculty of the School of Mechanical Engineering has approved the following new course. This action is now submitted to the Engineering Faculty with a recommendation for approval.

ME 53900 Introduction to Scientific Machine Learning, Sem. 1, alternate years, Class 3, cr. 3.
Prerequisites: None

Introduction to the fundamentals of predictive modeling for advanced undergraduates and graduate science and engineering students that work in the intersection of data and theory. Students who complete this course will be able to 1) represent mathematically the uncertainty in parameters of physical models; 2) propagate parametric uncertainty through physical models to quantify the induced uncertainty in quantities of interest; 3) calibrate the uncertain parameters of physical models using experimental data; 4) combine multiple sources of information to enhance the predictive capability of models; 5) pose and solve design optimization problems under uncertainty involving expensive simulations or experiments; 6) improve scientific writing and visualization skills.

Reason: This course has been taught two times on an experimental basis under the title “Introduction to Uncertainty Quantification” with the following enrollments: spring 2016 – 25 students, and spring 2018 – 40 students. The enrolled student population covered many engineering fields (mechanical, civil, aero, chemical, electrical, agricultural) along with some scientific fields (mathematics, statistics, atmospheric sciences). The course serves as a foundational course on data analytics and uncertainty quantification for engineering and science students. The intention is to co-list the course with Mathematics since it typically gets about 10 students from mathematics and statistics and it could also serve as a mathematics equivalent for engineering students. Video lectures of this course have been posted on NanoHUB.org and the intention is to create a digital version that is available to professionals. Note that the new title is compatible with the content of the course. The change in name is requested to make the course more attractive to professionals.

Eckhard Groll

ME School Head

ME 53900
INTRODUCTION TO SCIENTIFIC MACHINE LEARNING

Course Outcomes [Related ME Program Outcomes in brackets]

1. Represent mathematically the uncertainty in the parameters of physical models. [1]
2. Propagate parametric uncertainty through physical models to quantify the induced uncertainty in quantities of interest. [1]
3. Calibrate the uncertain parameters of physical models using experimental data. [1]
4. Combine multiple sources of information to enhance the predictive capabilities of models. [1]
5. Pose and solve design optimization problems under uncertainty involving expensive simulations or experiments. [1, 2]
6. Improve scientific writing and data visualization skills. [3]

Probability Theory (3 wks)

1. Random variables, expectations, conditional probabilities.
2. Common probability distributions/densities and their properties.
3. Random number generation. Rejection sampling. Inverse sampling.
4. Bayes' rule, parameter estimation, hypothesis testing, model selection.

Representation of Uncertainties (3 wks)

1. Generic principles. Invariant probabilities. Maximum entropy principle.
2. Dimension reduction. Principal component analysis. Non-linear dimensionality reduction methods.
3. Functional uncertainty. Random fields. Gaussian processes. Covariance functions. Karhunen-Loève expansion of random fields.

Uncertainty Propagation (3 wks)

1. Sampling methods. Monte Carlo, quasi-random sequences, Latin hypercube designs, multi-level Monte Carlo. Sobol sensitivity indices.
2. Classic collocation methods: Generalized polynomial chaos, sparse grid collocation.
3. Bayesian collocation methods: Bayesian linear regression, Gaussian process regression.

Calibration of Physical Models (2 wks)

1. Classical approach via minimization of (regularized) loss functions. Statistical (Bayesian) interpretation of the model calibration problem.
2. Sampling methods: Markov Chain Monte Carlo, Metropolis-Hastings, Hybrid Monte Carlo, Sequential Monte Carlo.
3. Variational methods: Automatic differentiation variational inference.

Optimization Under Uncertainty (2 wks)

1. Robust optimization, risk quantification, multi-objective optimization, Pareto-front, utility theory.
2. Bayesian global optimization: Probability of improvement, expected improvement, knowledge gradient.

COURSE NUMBER: ME 53900

COURSE TITLE: Introduction to Scientific Machine Learning

REQUIRED COURSE OR ELECTIVE COURSE: Elective

TERMS OFFERED: Spring, alternate years

TEXTBOOK/REQUIRED MATERIAL: None

PRE-REQUISITES: None

COORDINATING FACULTY: I. Bilionis

COURSE DESCRIPTION:
Introduction to the fundamentals of predictive modeling for advanced undergraduates and graduate science and engineering students that work in the intersection of data and theory.

ASSESSMENTS TOOLS:
1. In-class activities and quizzes.
2. Bi-weekly homework.
3. Project reports (initial, midterm, and final).

PROFESSIONAL COMPONENT:
None

NATURE OF DESIGN CONTENT:

Design optimization via the formulation of optimization problems under uncertainty. The focus is on the development of methodologies that can solve the design optimization problem with limited computational and experimental resources.

COMPUTER USAGE: All class activities, quizzes, homework, and the project require students to write Python code in the form of Jupyter notebooks

COURSE STRUCTURE/SCHEDULE:
1. Lecture – 2 days per week at 75 minutes.

COURSE OUTCOMES [Related ME Program Outcomes in brackets]:

1. Represent mathematically the uncertainty in the parameters of physical models. [1]
2. Propagate parametric uncertainty through physical models to quantify the induced uncertainty in quantities of interest. [1]
3. Calibrate the uncertain parameters of physical models using experimental data. [1]
4. Combine multiple sources of information to enhance the predictive capabilities of models. [1]
5. Pose and solve design optimization problems under uncertainty involving expensive simulations or experiments. [1, 2]
6. Improve scientific writing and data visualization skills. [3]

RELATED ME PROGRAM OUTCOMES:
1. Engineering fundamentals
2. Engineering design
3. Communication skills

PREPARED BY: I. Bilionis

REVISION DATE: 11 / 2020