The Hong Kong University of Science and Technology

UG Course Syllabus

Data Science for Molecular Engineering

CENG3300/BIEN3300

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Pre-requisites: CENG2310/BIEN2310

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Course Description

With the explosion of information and fast development of AI technologies, data science has become an essential skill for scientists and engineers in various fields. While molecular engineering is a subject that heavily engages data collection, processing and analytics, data science is not systematically included in the curriculum. This course introduces the basics of data science in the context of molecular engineering, which is in particular relevant to BIEN, CENG, CEEV students. It aims to provide students with the necessary knowledge and skill sets to dig into masses amount of science and engineering data, with applications in rational experimental design, molecular discovery and optimization, and predictive modeling, etc. These are important preparations for the students to take more advanced data science courses, as well as take on challenges in their future careers.

Intended Learning Outcomes (ILOs)

By the end of this course, students should be able to:

1. Identify problems that can be formulated as a supervised learning task
2. Process different types of data to be ready for model training
3. Understand the principles of supervised learning methods
4. Perform model training, validation and testing
5. Clearly interpret model predictions and present model results
6. Know the application of data science methods in molecular science related problems

Assessment and Grading

This course will be assessed using criterion-referencing and grades will not be assigned using a curve. Detailed rubrics for each assignment are provided below, outlining the criteria used for evaluation.

Assessments:

Assessment Task	Contribution to Overall Course grade (%)	Details
Homework	20%	Practice problems
Participation	10%	In-class activity participation
Course project	30%	Problem solving and presentation
Final examination	40%	Comprehensive assessment

Mapping of Course ILOs to Assessment Tasks

[add to/delete table as appropriate]

Assessed Task	Mapped ILOs	Explanation
Homework	ILOs 2, 3, 4, 5	This task assesses students' ability to technically perform data processing, analysis, model training and results presentations (ILOs 2, 3, 4 and 5)
Participation	ILOs 2, 3, 4, 5	Participation in in-class activities enhances understandings of concepts as well as practices the methods learned (ILOs 2, 3, 4 and 5)
Course project	ILOs 1, 2, 3, 4, 5, 6	The course project practice real world problem solving skills (ILOs 1 and 6), and reinforces technical skills (ILOs 2, 3, 4 and 5)
Final examination	ILOs 1, 2, 3, 4, 5	The final exam comprehensively assesses the technical side, including problem formulation (ILO 1) and problem solving. (ILOs 2, 3, 4 and 5)

Grading Rubrics

Homeworks and final exam will be graded based on technical correctness.

Participation will be graded based on the level of participation in in-class activities.

Course project will be graded based on the completeness of the project materials and quality of the presentation.

Final Grade Descriptors:

Grades	Short Description	Elaboration on subject grading description
A	Excellent Performance	Demonstrates a comprehensive grasp of subject matter, expertise in problem-solving, and significant creativity in thinking. Exhibits

		a high capacity for scholarship and collaboration, going beyond core requirements to achieve learning goals.
B	Good Performance	Shows good knowledge and understanding of the main subject matter, competence in problem-solving, and the ability to analyze and evaluate issues. Displays high motivation to learn and the ability to work effectively with others.
C	Satisfactory Performance	Possesses adequate knowledge of core subject matter, competence in dealing with familiar problems, and some capacity for analysis and critical thinking. Shows persistence and effort to achieve broadly defined learning goals.
F	Fail	Demonstrates insufficient understanding of the subject matter and lacks the necessary problem-solving skills. Shows limited ability to think critically or analytically and exhibits minimal effort towards achieving learning goals. Does not meet the threshold requirements for professional practice or development in the discipline.

Course AI Policy

Generally, responsible use of generative AI to complete course assignments is permitted. Exceptions will be mentioned in class.

Communication and Feedback

Assessment marks for individual assessed tasks will be communicated via Canvas within two weeks of submission. Feedback on assignments will include [specific details, e.g., strengths, areas for improvement]. Students who have further questions about the feedback including marks should consult the instructor within five working days after the feedback is received.

Academic Integrity

Students are expected to adhere to the university's academic integrity policy. Students are expected to uphold HKUST's Academic Honor Code and to maintain the highest standards of academic integrity. The University has zero tolerance of academic misconduct. Please refer to Academic Integrity | HKUST – Academic Registry for the University's definition of plagiarism and ways to avoid cheating and plagiarism.