Annexe A: New/Revised Course Content in OBTL+ Format

Course Overview

Expected Implementation in Academic Year	AY2019-2020
Semester/Trimester/Others (specify approx. Start/End date)	Semester 1
Course Author * Faculty proposing/revising the course	Lu Yunpeng
Course Author Email	yplu@ntu.edu.sg
Course Title	Artificial Intelligence In Chemistry
Course Code	CM4044
Academic Units	3
Contact Hours	62
Research Experience Components	Not Applicable

Course Requisites (if applicable)

Pre-requisites	PS0001 and PS0002, or CH2107 & CB0494 or by permission
Co-requisites	
Pre-requisite to	
Mutually exclusive to	
Replacement course to	
Remarks (if any)	

Course Aims

This course aims to equip you with working knowledge of how artificial intelligence (AI) can be applied to chemistry. As a start, you will learn the rigorous way to construct Python projects for AI. Next, you will learn how to apply AI to analyze chemical data, either for visualization, classification, quantitative determination, or for pursuing insights into chemical process. We will introduce multiple case studies and analyze how AI has impacted the various sub-disciplines of chemistry. The course will improve your communication skills by requiring you to deliver technical presentations to a broad audience. As a result of this course, you will develop the necessary skills to prepare yourself for a career that involves harnessing AI for research and industry applications

Course's Intended Learning Outcomes (ILOs)

Upon the successful completion of this course, you (student) would be able to:

ILO 1	Use Numpy or other similar packages for scientific computation
ILO 2	Use Matplotlib or other similar packages for scientific data visualization
ILO 3	Use Regular Expression or other similar packages for pattern searching in text information for data extraction
ILO 4	Use Pandas or other equivalent packages to load different format of data for analysis
ILO 5	Identify the functionalities in scikit-learn and other equivalent package
ILO 6	Apply scikit-learn or other package to build machine learning model
ILO 7	Identify the relevant functionalities in TensorFlow or other equivalent package
ILO 8	Build deep learning models by using TensorFlow or other equivalent/variant package
ILO 9	Identify interesting data-driven questions in chemistry.
ILO 10	Formulate meaningful study problems that you want to explore in chemistry
ILO 11	Collect/extract relevant data, visualize and perform exploratory analysis on data.
ILO 12	Perform machine learning models to extract meaningful insights from data.
ILO 13	Implement above techniques with Python
ILO 14	Present your analysis results and problem solution via an engaging written communication.

Course Content

Python Packages for Data Science and AI

1. Introduction to numpy package

2. Introduction to matplotlib package

3. Introduction to regular expression package

4. Introduction to Pandas package

5. Introduction to scikit-learn package

6. Introduction to TensorFlow package

AI applications in Chemistry

7. Data in chemistry: Data source, format and extraction

8. Introduction to data-driven scientific questions in chemistry

9. Visualization of chemical data and simple analysis based on primitive methods

10. Machine learning applications to data analysis in chemistry

11. Deep learning in data analysis in chemistry

Reading and References

1. Stuart Russell and Peter Norvig (2016) Artificial Intelligence: A Modern Approach, 3rd edition. Pearson. ISBN-13: 978-0136042594

2. Hugh Cartwright (2008) Using artificial intelligence in chemistry and biology: a practical guide,1st edition. CRC Press. ISBN: 9780849384141, 0849384141

3. Aurélien Géron (2017) Hands-On Machine Learning with Scikit-Learn and TensorFlow, 1st edition. O'Reilly. ISBN-13: 978-1-4919-6229-9

4. Hugh Cartwright (2003) Applications of artificial intelligence in chemistry, 1st edition, Oxford University Press. ISBN 019855737X, 0198557361

5. Rajarshi Guha and Andreas Bender (2012) Computational approaches in cheminformatics and bioinformatics, Wiley InterScience. ISBN: 9781118131411, 111813141x

Planned Schedule

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
1	Introduction to Numpy in scientific computing	1	Study several program using numpy package		Students will be asked to develop their simple program in lab tutorials
2	Introduction Matplotlib in data visualization	2	Study several program using Matplotlib package		Students will be asked to develop their simple program in lab tutorials.
3	Introduction to Regular Expression in pattern searching in text for data	3	Study several program using Regular Expression package		Students will be asked to develop their simple program in lab tutorials.
4	Introduction to Pandas package	4	Study several program using Pandas package		Students will be asked to develop their simple program in lab tutorials.
5	Introduction to scikit-learn package in machine learning	5,6	Study several program using scikit-learn package in machine learning		Students will be asked to develop their simple program in lab tutorials.
6	Introduction to tensorflow package in deep learning	7,8	Study several program using tensorflow package in machine learning		Students will be asked to develop their simple program in lab tutorials.
7	Data in chemistry	9	Lecture notes and reference books of Rajarshi Guha and Andreas Bender (2012) and Hugh Cartwright (2008).		Students will discuss about general concept of data and the specialty of chemical data. They will also learn to how to retrieve data from different sources

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
8	Introduction to data-driven scientific questions in chemistry	9, 10	Lecture notes, reference books of Rajarshi Guha and Andreas Bender (2012) and Hugh Cartwright (2008).		Students will discuss the concept of cheminformatics, particularly, in quantitative structure-activity relation and molecular descriptor in lab tutorial.
9	Machine learning examples in chemistry	1-6, 9-13	Lecture notes, reference books of Rajarshi Guha and Andreas Bender (2012) and Hugh Cartwright (2008).		Group project will be assigned. Lab practice on several machine learning models on chemical data
10	deep learning in chemistry	1-4, 7-13	Lecture notes, reference books of Rajarshi Guha and Andreas Bender (2012) and Hugh Cartwright (2008).		More group project will be assigned for deep learning Lab practice on several deep learning models on chemical data
11	Group Project	1-13			Group discussion on the project and collaborative work.
12	Group Project Presentations	14			Both lecture and lab tutorial time will be used for project presentation.

Learning and Teaching Approach

Approach	How does this approach support you in achieving the learning outcomes?
Lectures	Present the key ideas and important steps used to solve different types of problems
Lab Tutorials	Develop proficiency in problem solving skills. Reinforce concepts already covered in the lectures. Give an opportunity for weaker or more reserved students to clarify doubts.
Group projects	Train the class on teamwork and cohesion, as well as to boost confidence for weaker students. Develop communications skills. Students will be able to learn the importance of teamwork.

Assessment Structure

Assessment Components (includes both continuous and summative assessment)

No.	Component	ILO	Related PLO or Accreditation	Weightage	Team/Individual	Rubrics	Level of Understanding
1	Continuous Assessment (CA): Project(Group Projects)	All	Competence, Communication, Civic-mindedness, Character, Creativity.	40			
2	Continuous Assessment (CA): Assignment(Lab assignments)	All	Competence	20	Individual		
3	Continuous Assessment (CA): Others(Examination)	1-13	Competence, Creativity, Communication.	40	Individual		

Description of Assessment Components (if applicable)

Formative Feedback

You will receive written and verbal feedback from the lecturer for Components 2 & 3.

You will receive summative group feedback on the group project in component 1.

NTU Graduate Attributes/Competency Mapping

This course intends to develop the following graduate attributes and competencies (maximum 5 most relevant)

Attributes/Competency	Level
Collaboration	Intermediate
Communication	Intermediate
Digital Fluency	Advanced
Critical Thinking	Intermediate

Course Policy

Policy (Academic Integrity)

Good academic work depends on honesty and ethical behaviour. The quality of your work as a student relies on adhering to the principles of academic integrity and to the NTU Honour Code, a set of values shared by the whole university community. Truth, Trust and Justice are at the core of NTU's shared values. As a student, it is important that you recognize your responsibilities in understanding and applying the principles of academic integrity in all the work you do at NTU. Not knowing what is involved in maintaining academic integrity does not excuse academic dishonesty. You need to actively equip yourself with strategies to avoid all forms of academic dishonesty, including plagiarism, academic fraud, collusion and cheating. If you are uncertain of the definitions of any of these terms, you should go to the academic integrity website for more information. On the use of technological tools (such as Generative AI tools), different courses / assignments have different intended learning outcomes. Students should refer to the specific assignment instructions on their use and requirements and/or consult your instructors on how you can use these tools to help your learning. Consult your instructor(s) if you need any clarification about the requirements of academic integrity in the course.

Policy (General)

You are expected to complete all assigned pre-class readings and activities, attend all tutorial classes punctually and take all scheduled assignments and tests by due dates. You are expected to participate in all tutorial discussions and activities.

Policy (Absenteeism)

Absence from the midterm without a valid reason will affect your overall course grade. Valid reasons include falling sick supported by a medical certificate and participation in NTU's approved activities supported by an excuse letter from the relevant bodies. There will be no make-up opportunities for CA components.

All project assignments must be submitted on time. Failure to do so will affect your score.

Policy (Others, if applicable)

Appendix with Rubric (Assessment Criteria)

Please remember to attach the Appendix with Rubric (Assessment Criteria) if you have uploaded any.
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