University of California, Riverside
College of Natural & Agricultural Sciences
Artificial Intelligence in Toxicology and Environmental Health

Course Number: ENSC XXX/ ENTX XXX
Quarter: Fall XXXX
Units: 4 (Lecture: 3 hours; Discussion: 1 hour)
Lecture: M, W, F XX PM – XX PM (Location xxx)
Discussion: F XX PM – XX PM (Location xxx)

Instructor: Wei-Chun Chou, PhD
Office: XXX, Room xxx
Office hours: XXX
Email Address: XXX@ucr.edu

Class Q&A Platform
https:// xxxxxx/ucr/fallXXX/xxxxxxxxxxxxx

I. PURPOSE AND OUTCOME

Course Overview. This course will discuss fundamental principles, methodology and leveraging machine learning and artificial intelligence (AI) to investigate critical research questions within the fields of toxicology and environmental health. The students will explore cutting-edge techniques and tools based on machine learning and AI algorithms, including Physiologically based Physiologically Based Pharmacokinetic (PBPK) modeling, Quantitative Structure-Activity Relationship (QSAR) modeling for toxicity prediction, and comprehensive assessments of air pollution and ecotoxicology.

Relation to Program Outcomes. This course bridges the realms of AI with environmental toxicology, ecotoxicology, and environmental health, offering invaluable insights and skills to students in our environmental toxicology graduate program. It equips them with quantitative modeling, advanced machine learning, and artificial intelligence tools to assess the impact of environmental chemicals on ecological systems, human health, and environmental health. Our course distinguishes itself from other courses offered by addressing an emerging field, including extensively exploring the application of machine learning and AI in toxicology and environmental health, which has not been thoroughly discussed in existing courses.

Course Objectives. This course has the objective to provide students with a conceptual understanding of fundamental AI methods, including practical examples in toxicology and environmental health, and to get them acquainted with high-level AI algorithms by Python for data analysis and visualization. Upon successful completion of this course, students will be able to:

- **Comprehensive Understanding**: Develop a comprehensive understanding of fundamental AI methods and their practical applications in the fields of toxicology and environmental health.
- **Research Topics Familiarization:** Familiarize students with various research topics within toxicology and environmental health that can be effectively studied using machine learning and artificial intelligence approaches.

- **Critical Analysis Skills:** Enable students to critically evaluate different machine learning and AI methodologies when addressing specific research questions in toxicology and environmental health, empowering them to select the most optimal approach.
- **Strengths and Limitations Assessment:** Equip students with the ability to assess the strengths and limitations of studies applying machine learning and artificial intelligence to investigate toxicology and environmental health research problems.
- **Research Design and Implementation with AI methods**: Develop students' research design and execution skills, allowing them to conduct studies that employ appropriate machine learning and AI techniques to investigate chemical exposure, toxicokinetics, toxicity, risk assessment, and their impacts on human and environmental health.

Instructional Methods. This course is offered weekly, in person. The instructional methods will include assigned readings, lectures, computational modeling and analysis demos using a recent publication as a case study, student presentations, class discussions, and assignments.

1. **Assigned Homework Assignments:** Weekly homework assignments will be provided to students to promote a deeper understanding and facilitate their learning process.
2. **Lectures:** Weekly lectures will introduce the core principles of applying different machine learning and artificial intelligence methods to diverse toxicology and environmental health research questions.
3. **Computational Modeling Analysis Demos:** Lectures will also include demonstrations illustrating how to conduct computational modeling and analysis, with a focus on reproducing results from recent publications as case studies.
4. **Student Presentations and Class Discussion:** Each week, a designated student will have the opportunity to present a recent publication, offering insights into the strengths, limitations, and applications of machine learning and artificial intelligence approaches, along with highlighting the major findings. This presentation sets the stage for in-depth discussions in the section, where students can share relevant comments and engage in a dynamic exchange of ideas about the topics.

II. DESCRIPTION OF COURSE CONTENT

Topical Outline/Course Schedule

Tentative class schedule:

Week	Lecture	Date(s)	Topic(s)	Reference Text
0	1	XXX	**Course Introduction and Overview**	
1	2	XXX	**Fundamental Concepts of Machine Learning and Artificial Intelligence** ● Fundamental Concepts of Machine Learning and Artificial Intelligence ● Basic Coding Examples of Machine Learning and Artificial Intelligence	Lin and Chou (2022) Chapter 1-3 in Geron (2019)
	3	XXX		
	4	XXX		

Week	Lecture	Date(s)	Topic(s)	Reference Text
2	5	XXX	**Intuitive Explanation of Machine Learning Methods –Part 1** ● Commonly Used Machine Learning Approaches – Part 1 ● Hands-on Exercise: End-to-End Machine Learning Project 1	Chapters 4 and 5 in Geron (2019)
	6	XXX		
	7	XXX		
3	8	XXX	**Intuitive Explanation of Machine Learning Methods –Part 2** ● Commonly Used Machine Learning Approaches in Environmental and Global Health – Part 2 ● Hands-on Exercise: End-to-End Machine Learning Project 2	Chapters 6 and 7 in Geron (2019)
	9	XXX		
	10	XXX		
4	11	XXX	**Intuitive Explanation of Machine Learning Methods –Part 3** ● Commonly Used Machine Learning Approaches in Environmental and Global Health – Part 3 ● Hands-on Exercise: End-to-End Machine Learning Project - Part 3	Chapters 10 and 11 in Geron (2019)
	12	XXX		
	13	XXX		
5	----	XXX	**Review** ● Review Lecture 1 – Lecture 13 **Midterm exam**	
	----	XXX		
6	14	XXX	**AI in Absorption, Distribution, Metabolism, and Excretion (ADME)** ● Roles of Machine Learning and Artificial Intelligence for ADMET Profiling ● Build a Simple QSAR Model to Predict the Plasma Half-life of Chemicals	Chapter 8 in Ekins (2018)
	15	XXX		
	16	XXX		
7	17	XXX	**AI in Physiologically Based Pharmacokinetic (PBPK) Modeling** ● Roles of Machine Learning and Artificial Intelligence in PBPK Modeling ● Build an AI-based PBPK for Nanoparticles	Chou and Lin (2023) Chou et al. (2023)
	18	XXX		
	19	XXX		

Week	Lecture	Date(s)	Topic(s)	Reference Text
8	20	XXX	**AI in Quantitative Structure-Activity Relationship (QSAR)** ● Molecular Descriptors for Quantitative Structure-Activity Relationship (QSAR) Modeling ● Roles of Machine Learning and Artificial Intelligence in the Prediction of Human Toxicity ● Build a QSAR Model to Predict Organ Toxicity	Chapters 1 and 2 in Nicolotti (2018) OECD (2014) Xu et al. (2022)
	21	XXX		
	22	XXX		
9	23	XXX	**AI in environmental chemistry and ecotoxicology** ● Roles of Machine Learning and Artificial Intelligence in Predicting Transport, Transformation, or Removal of Chemicals in soil, water, and air. ● Build a Simple Machine Learning Model to Predict the Impact of Chemicals on Ecological Systems.	Chen et al. (2023) Song et al. (2022)
	24	XXX		
	25	XXX		
10	26	XXX	**AI in Health Outcome of Air Pollution** ● Roles of Machine Learning and Artificial Intelligence in Predicting Health Outcomes of Air Pollution ● Build a Simple Machine Learning Model to Predict the Health Outcome of Air Pollution	Lee et al. (2022) Coker et al. (2022)
	27	XXX		
	28	XXX		
FINAL EXAM				

III. Weekly Discussion Topics

Week	Date(s)	Topic(s)	Reference
0	XXX	**Unveiling Artificial Intelligence: Transforming Our Daily Lives**	Chapter 1 in Geron (2019)
1	XXX	**Exploring Fundamentals in Machine Learning and Artificial Intelligence**	Chapters 1-3 in Geron (2019)
2	XXX	**Discussing the Concept of the Common-Use Machine Learning Methods: Use a Support Vector Machine as an example**	Chapters 4 and 5 in Geron (2019)
3	XXX	**Discussing the Concept of the Common-Use Machine Learning Methods: Use a Random Forest as an Example**	Chapters 6 and 7 in Geron (2019)

Week	Date(s)	Topic(s)	Reference
4	XXX	**Discussing the Concept of Deep Neural Network**	Chapters 10 and 11 in Geron (2019)
5	XXX	**Review Homework Problem Sets**	----
6	XXX	**CASE STUDY 1**	AI in the Prediction of ADME of Chemicals
7	XXX	**CASE STUDY 2**	AI in PBPK model
8	XXX	**CASE STUDY 3**	QSAR model for Toxicity predictions
9	XXX	**CASE STUDY 4**	AI Models Used in Ecotoxicology
10	XXX	**CASE STUDY 5**	AI Models Used in the Air Pollution

IV. COURSE MATERIALS

Course slides. Provided by the course instructor and posted online.

Textbook(s):

Aurélien Géron. Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow. **2nd** Edition. 201**9**. O'Reilly Media, Inc. Available online (UCR campus/VPN) at https://github.com/ageron/handson-ml2

Gareth James, Daniela Witten, Trevor Hastie, Robert Tibshirani. (2013). An introduction to statistical learning: with applications in R. New York: Springer. Available online (UCR campus/VPN) at https://www.statlearning.com/

Reading materials. Nonmandatory.

Chen H, Zheng Y, Li J, Li L, Wang X. AI for Nanomaterials Development in Clean Energy and Carbon Capture, Utilization and Storage (CCUS). ACS Nano. 2023 Jun 13;17(11):9763-9792. doi: 10.1021/acsnano.3c01062. Epub 2023 Jun 2. PMID: 37267448.

Chou WC, Chen Q, Yuan L, Cheng YH, He C, Monteiro-Riviere NA, Riviere JE, Lin Z. An artificial intelligence-assisted physiologically-based pharmacokinetic model to predict nanoparticle delivery to tumors in mice. J Control Release. 2023, 361:53-63.

Chou WC, Lin Z. Machine learning and artificial intelligence in physiologically based pharmacokinetic modeling. Toxicological Sciences. 2023, 191(1):1-14.

Coker ES, Buralli R, Manrique AF, Kanai CM, Amegah AK, Gouveia N. Association between PM2.5 and respiratory hospitalization in Rio Branco, Brazil: Demonstrating the potential of low-cost air quality sensor for epidemiologic research. Environ Res. 2022, 214(Pt 1):113738.

Ekins S. Computational Toxicology: Risk Assessment for Chemicals. 2nd Edition. Wiley Series on Technologies for the Pharmaceutical Industry Ser. 2018. Pages: 1-425.
Geron A. Hands-on machine learning with Scikit-Learn, Keras & TensorFlow: Concepts, Tools, and Techniques to Build Intelligent Systems. Second Edition. 2019, 1-484
Lee ES, Kim JY, Yoon YH, Kim SB, Kahng H, Park J, Kim J, Lee M, Hwang H, Park SJ. 2022. A Machine Learning-Based Study of the Effects of Air Pollution and Weather in Respiratory Disease Patients Visiting Emergency Departments. Emergency Medicine International. 2022, 2022:4462018.
Lin Z, Chou WC. Machine learning and artificial intelligence in toxicological sciences. Toxicological Sciences. 2022, 189(1):7-19.
Nicolotti O. Computational Toxicology: Methods and Protocols. 1st Edition. Springer Nature. 2018. Pages: 1-587.
OECD (2014), Guidance Document on the Validation of (Quantitative) Structure-Activity Relationship [(Q)SAR] Models, OECD Series on Testing and Assessment, No. 69, OECD Publishing, Paris, https://doi.org/10.1787/9789264085442-en.
Song R, Li D, Chang, A. et al. Accelerating the pace of ecotoxicological assessment using artificial intelligence. 2022. Ambio 51, 598–610.
Xu M, Yang H, Liu G, Tang Y, Li W. In silico prediction of chemical aquatic toxicity by multiple machine learning and deep learning approaches. J Appl Toxicol., 2022, 42(11):1766-1776.

V. GRADING AND COURSE REQUIREMENTS

Learning assessment methods: Students will be graded with the following four learning assessment methods.

1. **Weekly Quizzes (70 points, 14% of total points)**: Weekly quizzes, except for the first week, will assess students' comprehension of the theoretical course content. Each quiz will consist of 5 single-choice or multiple-choice questions, accounting for 5 points. In total, these quizzes will contribute to 70 points over 10 weeks.
2. **Homework assignments (140 points, 28% of total points)**: Throughout the quarter, you will receive homework problem sets to enhance your understanding of the course material. Collaborating with your peers is encouraged to facilitate learning. It is crucial to submit your homework assignments punctually, as late submissions will incur a 10% deduction from the total possible points for each day of delay. A strong grasp of these problem sets is pivotal in solidifying your comprehension of the subject matter and equipping you for success in the exams.
3. **Journal Presentations (140 points, 28% of total points)**: Similar to journal reviews, students will lead one or two weekly journal presentations, depending on class size. Instructors will assign presenters and provide journal papers one week in advance.
4. **Mid-Term and Final Exams (75 points for the mid-term exam and 75 points for the final exam, 30% of total points)**: Both the mid-term and final exams will be research problem-based assignments. Instructors will select recent publications related to the application of AI methods in toxicology and environmental health sciences, such as PBPK, QSAR, air pollution, and ecotoxicology assessment. Students will use model code from supplementary materials provided by instructors to answer 3-5 specific

challenging questions. Exams will be posted one week before the due date, allowing sufficient time for completion.

VI. GRADING SCALES

A = 94-100%; A- = 90-93%;
B+ = 87-89%; B = 84-86%; B- = 80-83%;
C+ = 77-79%; C = 74-76%; C- = 70-73%;
D+ = 67-69%; D = 64-66%; D- = 60-63%;
F = <60%

VII. POLICIES AND PROCEDURES

Academic Integrity: The University of California, Riverside has clearly articulated its policies governing academic integrity and students are encouraged to carefully review the Academic Integrity Policies and Procedures at https://conduct.ucr.edu/policies/academic-integrity-policies-and-procedures. Any deviation from these expectations will result in academic penalties as well as disciplinary action. The area of greatest potential risk for inadvertent academic dishonesty is plagiarism. Plagiarism includes but is not limited to, paraphrasing or direct quotation of the published or unpublished work of another person without full and clear acknowledgement.

Attendance: Students are obligated to complete all assigned work promptly, to attend class regularly, and to participate in whatever class discussion may occur. Absence from more than 10 percent of the scheduled class sessions, whether excused or unexcused, is excessive. Although the instructor will not be monitoring attendance, a lack of attendance will adversely affect performance on all course requirements throughout the quarter. Students should meet with the instructor early in the quarter to discuss the consequences of potential excessive absences due to participation in University-sponsored events.

Classroom Behavior: Please be respectful of each other, the instructor, and any guest lecturers while in class. While laptops and tablets are permitted for taking notes during class, all cell phones and pagers are to be turned off or silenced during class (not on vibrate), and text messaging, web browsing, etc. during class is not permitted. Failure to adhere to these classroom rules may result in your being dismissed from class.

Communication: All announcements and communications between the instructor and students will occur via Canvas.

Disabilities: Reasonable accommodations are available for students with a documented disability. Please contact the Student Disability Resource Center (1228 Student Services Building; T: (951) 827-3861, E-mail: sdrc@ucr.edu) if you have a disability and need accommodations to fully participate in this class. More information is available at https://sdrc.ucr.edu/students-disabilities. All accommodations must be approved through the Student Disability Resource Center.

Diversity: Please respect each other's opinions and refrain from personal attacks or demeaning comments of any kind.

Instructor Expectations: The instructor is expected to facilitate learning, answer questions appropriately, be fair and objective in grading, provide timely and useful feedback on exams and papers, provide office hours, and treat students with respect.

Syllabus Amendments: The instructor reserves the right to make changes to the syllabus when unforeseen circumstances occur or we take longer than expected on certain subject matter. The changes will be announced as early as possible so that students can adjust their schedules. Amendments will be distributed in writing to all students via Canvas.