

Overview

Module Description

This module seeks to infuse experience with AI models into chemistry laboratory courses with the goal of training students on how to recognize AI works and how to responsibly and ethically utilize AI models in higher education. Students will undertake several modules where they will first use AI to compare its answers to the answers they come up for several problems, including some basic chemistry and math as well as some predictive work in an integrated research project part of the lab sequence. Students will then critique the effectiveness of the AI models in providing correct information as well as examine the methodology of the AI-generated responses. Finally, students will explore the potential uses and pitfalls of using predictive AI within the broader chemistry field (such as designing new molecules or protocols).¹ Discussion of ways that AI can specifically enhance knowledge in the field of chemistry² will be critical to developing new career tracks (mirrored by many universities cluster hiring of AI scientists³).

Learning Outcomes

- Students should recognize capabilities and limitations of AI models.
 - Recognize patterns in AI responses.
 - Examine veracity of answers provided.
- Students should be able to describe the ethical implications of using AI models in their work.
 - Can AI models assist them in learning? Designing quizzes, flashcards, mnemonics.
 - How can abusing AI for quick answers harm them, their peers, or others?
- Students should design processes to utilize AI models (current and future) to advance chemistry research.
 - Examine characteristics of soil types and ions to predict level of interaction.
 - Need for accessible data to train AIs.

Module Organization and Timeline

Class Discussion and Assessment on Topic #1: What is AI? How Can We Recognize It? (1 Week)

- During pre-lab discussion, talk about AI models and how they function. Include some demonstrations.
- Provide resources on Canvas discussing how AI models are trained and the basic ideas of the parameters they use to construct responses.
 - <https://ecraft2learn.github.io/ai/>
 - <https://viso.ai/deep-learning/ml-ai-models/>
- Have students take AI quiz(es) and report their results and impressions on a discussion board.
 - <https://roft.io/>

¹ Artificial Intelligence in Chemistry: Current Trends and Future Directions. Zachary J. Baum, Xiang Yu, Philippe Y. Ayala, Yanan Zhao, Steven P. Watkins, and Qiongqiong Zhou Journal of Chemical Information and Modeling 2021 61 (7), 3197-3212 DOI: 10.1021/acs.jcim.1c00619

² <https://thegradiant.pub/how-ai-is-changing-chemical-discovery/>

³ <https://www.insidehighered.com/news/2015/05/01/new-report-says-cluster-hiring-can-lead-increased-faculty-diversity>

- More Introduction
 - Pre-test on AI
 - Preferably as a Canvas quiz
 - Play around with some AIs
 - ChatGPT
 - Bard
 - Claire
 - More – <https://intellipaat.com/blog/top-artificial-intelligence-tools/>
 - Play around with some bias training
 - Harvard test
 - Trainable Machine

Class Discussion and Assessment on Topic #2: What are the Ethical Concerns Centered around AI Use? (3 Weeks)

- Demonstrate in pre-lab answering some chemistry questions with AI models.
- Class discussion on ethics of using AI to get answers
 - Safety of AI – <https://scottaaronson.blog/?p=6823>
 - <https://teaching.cornell.edu/generative-artificial-intelligence/ethical-ai-teaching-and-learning>
- Have students look for patterns in AI responses (similar to week 3 quiz)
 - <https://www.technologyreview.com/2022/12/19/1065596/how-to-spot-ai-generated-text/>
- Ask students to craft their own questions and answer them in AI model of their choice and share results on Discussion board
 - <https://ditchthattextbook.com/ai-tools/>
 - <https://www.tryinteract.com/blog/make-a-quiz-with-openai-chatgpt/#assessment>

More Ethics

- Montreal Declaration (<https://montrealdeclaration-responsibleai.com/the-declaration/>)
 - Equity – how does AI use affect overall test scores? Competition for limited positions (professional schools)
 - Prudence – does AI give valid answers? Can it address specific problems and account for variables?
 - Responsibility – if you use AI and it provides an errant response, who is to blame?
- What are the stakes for relying on AI?

- No power – what do you do?
- Unusual case – can you oversee/troubleshoot the response? (X-Files – Fight the Future)
- Discussion of Ethical Concerns
 - [Montreal protocols](#)
 - [UNESCO](#)

Class Discussion and Assessment on Topic #3: How Can We Responsibly Use AI in Chemistry? (3 Weeks)

- Discussion of chemistry-specific applications of AI models
 - Protein structure and availability of PDB (<https://www.rcsb.org/>)
 - Comparison of PDB with many chemistry datum being sequestered in journals, often behind paywalls and the difficulty of accessing enough data to properly train an AI for a specific task
- Ethical discussion of who owns the data? How should access be governed?
 - In-class and Discussion Board responses
- Wrapping Up
 - Post-test on Canvas
 - Can students use AI to generate a study guide for the last exam?
 - How useful are AI tools in answering Lab Questions?

Each topic is designed to take about 20-30 minutes of class time.

- Out of class readings/quizzes.
- In-class lectures, discussion, and examples

Assessment Rubric

The student's work will be assessed using the AAC&U Ethical Reasoning VALUE Rubric available at VALUE Rubrics - Ethical Reasoning | AAC&U (aacu.org)

For this course, different different evaluation criteria were applied for different assignments. For convenience, the AACU Value Rubric is also provided below:

ETHICAL REASONING VALUE RUBRIC

for more information, please contact value@aacu.org



Definition

Ethical Reasoning is reasoning about right and wrong human conduct. It requires students to be able to assess their own ethical values and the social context of problems, recognize ethical issues in a variety of settings, think about how different ethical perspectives might be applied to ethical dilemmas, and consider the ramifications of alternative actions. Students' ethical self-identity evolves as they practice ethical decision-making skills and learn how to describe and analyze positions on ethical issues.

Evaluators are encouraged to assign a zero to any work sample or collection of work that does not meet benchmark (all one) level performance.

| | Capstone 4 | Milestones 3 2 | | Benchmark 1 |
|--|--|---|--|--|
| Ethical Self-Awareness | Student discusses in detail/analyzes both core beliefs and the origins of the core beliefs and discussion has greater depth and clarity. | Student discusses in detail/analyzes both core beliefs and the origins of the core beliefs. | Student states both core beliefs and the origins of the core beliefs. | Student states either their core beliefs or articulates the origins of the core beliefs but not both. |
| Understanding Different Ethical Perspectives/Concepts | Student names the theory or theories, can present the gist of said theory or theories, and accurately explains the details of the theory or theories used. | Student can name the major theory or theories she/he uses, can present the gist of said theory or theories, and attempts to explain the details of the theory or theories used, but has some inaccuracies. | Student can name the major theory she/he uses, and is only able to present the gist of the named theory. | Student only names the major theory she/he uses. |
| Ethical Issue Recognition | Student can recognize ethical issues when presented in a complex, multilayered (gray) context AND can recognize cross-relationships among the issues. | Student can recognize ethical issues when issues are presented in a complex, multilayered (gray) context OR can grasp cross-relationships among the issues. | Student can recognize basic and obvious ethical issues and grasp (incompletely) the complexities or interrelationships among the issues. | Student can recognize basic and obvious ethical issues but fails to grasp complexity or interrelationships. |
| Application of Ethical Perspectives/Concepts | Student can independently apply ethical perspectives/ concepts to an ethical question, accurately, and is able to consider full implications of the application. | Student can independently (to a new example) apply ethical perspectives/ concepts to an ethical question, accurately, but does not consider the specific implications of the application. | Student can apply ethical perspectives/ concepts to an ethical question, independently (to a new example) and the application is inaccurate. | Student can apply ethical perspectives/ concepts to an ethical question with support (using examples, in a class, in a group, or a fixed-choice setting) but is unable to apply ethical perspectives/ concepts independently (to a new example). |
| Evaluation of Different Ethical Perspectives/Concepts | Student states a position and can state the objections to, assumptions and implications of and can reasonably defend against the objections to, assumptions and implications of different ethical perspectives/ concepts, and the student's defense is adequate and effective. | Student states a position and can state the objections to, assumptions and implications of, and respond to the objections to, assumptions and implications of different ethical perspectives/ concepts, but the student's response is inadequate. | Student states a position and can state the objections to, assumptions and implications of different ethical perspectives/ concepts but does not respond to them (and ultimately objections, assumptions, and implications are compartmentalized by student and do not affect student's position.) | Student states a position but cannot state the objections to and assumptions and limitations of the different perspectives/ concepts. |