PENNSYLVANIA BIOTECHNOLOGY CENTER

Est. by the Hepatitis B Foundation

Fall 2024

Artificial Intelligence for Science

Course Start Date: 09/17/2024
Course End Date: 10/24/2024

Course Director:

Jessica Freeze, PhD
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Office Hours: by appointment

Course Location/Format: Pennsylvania Biotechnology Center
3805 Old Easton Rd, Doylestown, PA 18902
Room 3100/In Person

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Contact Information

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Questions?
For administrative questions, please reach out to Dr. Freeze via her provided email. For class related questions (concepts, projects, homework, etc), please use the Google Classroom Forum.

Purpose of the Course Syllabus:

This syllabus is a guide detailing the expectations of the course faculty and requirements for successful completion of the Artificial Intelligence for Science course. Information in this syllabus is subject to change during the presentation of the course to accommodate unexpected emerging student need. Any changes in the course will be announced during the classroom session and will be emailed to the class list.

Course Description:

This course is designed to introduce artificial intelligence in the context of scientific application to high school students. The emphasis will be on the fundamentals of machine learning and how they can be applied to scientific study, and to prepare students for future success in science and engineering programs at college.

Topics will include the fundamentals defining artificial intelligence and its subfield of machine learning, with an emphasis on current methods and models and their use cases. Additional depth will be given to the area of deep learning, including the evolution of models and the mechanisms governing their training. Discussion of methods used to accelerate machine learning and experience using some of the latest tools will top off the first half of the course. The second half of the course will apply the lessons from the first half to display the applications of machine learning in the physical sciences, medicine, space exploration, and robotics. Key topics will include limitations guiding execution of AI tools in scientific study, ethical considerations, and the future of AI in science. Students should expect homework and projects to solidify and expand their lecture-based learning.

Required / Recommended Texts:

There will not be a required textbook for this course. Necessary materials will be provided in the form of handouts, URLs for pertinent web sites, or podcasts.

Recommended reference texts for Artificial Intelligence for Science include:

Michael A. Nielsen, "Neural Networks and Deep Learning", Determination Press, 2015 <http://neuralnetworksanddeeplearning.com>

US Department of Energy National Laboratory; Berkeley Lab; The University of California, "Machine Learning for Science", Berkeley Lab, <https://ml4sci.lbl.gov>

Machine Learning for Science Team, "Machine Learning for Scientists", Machine Learning for Science, <https://ml-lectures.org/docs/introduction/introduction.html>

Collaborative Teaching Model:

This course will be implemented using team-based teaching. Students will be instructed in course topics by multiple faculty members who are experienced in these areas. The course director is responsible for the administration of the course.

Course Materials and Forum:

Course materials, including lectures slides, homeworks, quizzes, and project details can be found on the Google Classroom course website. Questions about course topics and assignments can also be asked through the Google Classroom Stream/Forum.

Course Outcomes:

The goal of this course is to enable students to apply their knowledge of AI for science to better evaluate new AI/ML technologies and their uses in fields of science, as well as to prepare them for more advanced study at the college level.

Objectives:

By the end of this course students will be able to:

1. Understand the foundational principles of artificial intelligence.
2. Explore the intersection of AI with various scientific disciplines.
3. Recognize the potential and limitations of AI in scientific research and applications.
4. Develop hands-on experience with simple AI tools and projects.
5. Cultivate a critical mindset towards the ethical considerations and consequences of AI in science.

Course Outline and Corresponding Objectives:

Curriculum Week	Topic	Objectives
1a **9/17/2024**	Introduction to Machine Learning	Syllabus Intro; What is AI? Definition, what it isn't; AI vs. Human Intelligence – rationality, optimality, neuroscience; History of AI. – Expert models, step function, winter, sigmoid activation, timeline; Where does Machine Learning fit in AI? – Subset, Statistics, Agents; Types of Learning and Objectives
1b **9/19/2024**	Basic Principles of Machine Learning	Training a model; Non-Neural Network Models
2a **9/24/2024**	Neural Networks Overview	Neural Network Basics; Neural Network Models
2b **9/26/2024**	Building and understanding basic feed-forward networks	Coding a basic Machine Learning model in Python with/out ML libraries; Importance of data selection, generalization, and training procedures
3a **10/1/2024**	Limitations and Challenges of AI in Scientific Research	Data quality; Input representation impacts; Model structure impacts; Uncertainty in model output; Understandability of models; Impact of hallucinations; Current understanding bias; The importance of domain knowledge.
3b **10/3/2024**	AI/ML Accessories	Data Preprocessing – Images, Principal Component; Analysis, Removing outliers; Active Learning; Compute power; Retrieval Augmented Generation (RAG); LLMs
4a **10/8/2024**	AI in Physical Sciences	AI in Physics: Simulations and predictions. AI in Chemistry: Materials, spectra, and synthesis
4b **10/10/2024**	AI in Medicine	AI in drug discovery and molecular dynamics. Predictive modeling in genetics. AI in medical imaging and diagnosis.
5a **10/15/2024**	AI in Space Exploration and Astronomy	AI in satellite image analysis. Predicting celestial events.
5b **10/17/2024**	AI Agents for Robotic Action	What is an agent and what models guide agents The realities of online, real-time, embedded systems Current state of AI robots
6a **10/22/2024**	Ethical Considerations of AI in Science	Ethics 101; Ethical concerns and examples
6b **10/24/2024**	The Future of AI in Science	Quantum computing and AI. The potential of AI in unifying scientific theories. Reflect on the potential and challenges of integrating AI into future scientific endeavors. New technology enabling faster calculations/training. The Data Cliff

Instructional Methodology:

A combination of lectures, homework tutorials, and guided project-based learning will be implemented. Lecture materials will be made available through the class mailing list. Homework will be delivered to students at the end of the assigning class and due at the beginning of the next lecture through the class portal. Student participation will be required. A class Slack will be available for the duration of the course and may be used to ask questions and receive help with class material. It is expected that electronic and online content will serve to supplement the learning experience.

For this course, a combination of small group and self-directed learning will be used to help you accomplish the objectives. Students will be allowed to work with other students throughout this course but must outline their and their partners contributions on homework and project. The student is responsible for the competition of their own work. No copying is permitted.

Evaluation Methods:

Final course grades will be determined by performance on the class participation, quizzes, homework, and a final project presentation. Students will receive an anonymized student ID at the beginning of the course. Grades will be posted using these anonymous IDs through the class portal. Students may doublecheck their ID with the Course Director at any time through email or private message on Slack. Additional details on each metric are given below. The total grade must be greater than 70% for completion. Grades may be adjusted up on a curve at the end of the course, but will not be adjusted down.

Grading Policies:

Grades for this course will be given as a percentage to two decimal places. Completion of the course will be reflected through a completion certificate and digital badge on the student's LinkedIn account. To receive this certificate, the student's final curved grade must be >= 70.00%.

Post-Assignment Review and Grade Disputes:

If a homework or quiz question is found to have resulted in > 50% of assignment-takers selecting an incorrect answer, the course director will review with class either by discussion post or Zoom meeting. If additional help is needed, the student may request help from the class instructors through Slack.

Additionally, students may challenge an assignment grade/question within seven business days of the posting of the grade. The burden of proof for a challenge to the contrary rests with the student. The course director will respond to the student's challenge within seven business days of the receipt of dispute.

Percent weighting of each scored component of the course

Examination	% Weight	Additional Details
Quizzes	30	Will cover the previous week's material; 5 minutes each at the end of each (b) class; 5 multiple choice or fill in the blank questions each; Grades delivered next class via student id list – score sheet; Each quiz gets two chances – first time on the (b) class of the week, 2nd time on the (a) class of the following week. – Same quiz; Best of two quiz grades kept; Must receive an 80% overall on quizzes to get completion
Homework	30	10 homework assignments – Each worth 3%; Note, some nights have both homework and project expectations – these are graded separately.; Given after each class and due at the start of the next class through the class portal; Must submit at least 90% of homework for completion.
Project	30	Five project components – each worth 6%
Attendance	10	Students may not miss more than 2 lectures without proof of extenuating circumstance to qualify for completion.; Students should inform the professor as soon as possible, or within two business days (whichever is justifiably greater) of extenuating circumstances they wish to be excused of and to receive make-up work.; Each unexcused lecture (up to 2) missed will subtract 5% from the student's total uncurved score.

Course Evaluation Policy:

Course and faculty evaluations are an essential tool to provide feedback to course directors, enhance future renditions of a course, and aid the organization as it continues to constantly evolve its curriculum. Consequently, students are expected to complete all requested course and faculty evaluations as part of their homework grade and will not receive their final grade or completion certificate until the evaluations are complete.

Social Justice and Title IX Statement on Non-Discrimination

The instructors and course director are committed to providing an inclusive and welcoming environment and to ensuring that educational decisions are based on individuals' abilities. Consistent with these principles and applicable laws, it is therefore policy to not discriminate on the basis of age, color, disability, gender, gender expression, gender identity, genetic information, national origin, race, religion, sex, sexual orientation or veteran status. No person, on the basis of protected status, shall be excluded from participation in, be denied the benefits of, or be subjected to unlawful discrimination, harassment, or retaliation throughout this course.

Disability Support Services

If you are a person with a disability and anticipate needing any type of accommodation in order to participate in this class, please advise the course director. The course director will make all reasonable accommodations as available. Failure to notify the course director of such disability needs implies acceptance of conditions of the course.