《人工智能在科学与工程学的应用》教学大纲

一、课程基本信息

课程名称/英文名称	人工智能在科学与工程学的应用/AI for Science and Engineering	课程代码	CS286
课程层次	本研一体	学分/学时	4/64
主要面向专业	信息科学，物质科学，生命科学等理工科专业	授课语言	双语
先修课程		建议先修说明	Python 编程，概率统计，微积分，线性代数
开课单位	信息科学与技术学院	课程负责人	郑杰

注 1：课程层次填写“本科生课程”、“研究生课程”或“本研一体课程”

注 2：主要填写全校 10 个本科专业（或若干个专业的组合）或“全体本科生”或“全校学生”

注 3：显示课程信息里的“强制先修课程”信息，强制先修课程是本课程的选课强制约束条件；教师在录入课程教学大纲时，该信息显示但不可修改

注 4：可在此填写教师对学生修读本课程之前应具备哪些知识基础的建议

二、课程简介

近年来，由于大量科学数据的出现以及深度学习的迅猛发展和广泛应用，人工智能（Artificial Intelligence, 简称 AI）技术在科学和工程学研究中变得越来越重要。本课程的主要目标是使不同学术背景的学生能够在研究项目中理解和使用人工智能技术。在课堂讲授中，在介绍了人工智能方法的基础知识（尤其是深度学习）之后，将描述和解释人工智能在科学和工程领域的应用实例，包括但不限于材料科学、分子生物学、蛋白质工程、药物发现等。通过在教程、作业和课程项目中的实践练习，学生将能够使用最先进的人工智能技术解决具体的研究问题。此外，学生将能够开发新的人工智能技术，推动科学和工程领域的发展，为将来在各个领域中成功应用人工智能打下扎实的基础。

本课程的主要特色是实践项目驱动的学习法，强调动手能力的培养，将理论与实际应用紧密结合。因此，本课程的 4 个学分中，包含 2 个理论学分和 2 个实践学分。

三、课程教学目标

知识认知能力培养：通过本课程的学习，学生应该能够: （1）理解机器学习（尤其是深度学习）和其他人工智能技术的基本思想； （2）获得使用人工智能技术解决科学或工程问题的经验；（3）确定可以使用人工智能技术解决的研究问题；（4）针对给定的研究问题选择最适合的机器学习方法；（5）提出创新，以提高现有机器学习方法的性能，在准确性、计算效率等方面。

综合素质能力培养：这是一门科研导向的多学科交叉融合的课程。因此，通过学习本课程，学生将能够:（1）加强与不同背景的同学及研究人员的沟通能力；（2）培养创造性和综合思维能力，能够整合不同来源的知识和资源来解决问题；（3）掌握和提高使用计算机软件探索多模态数据的动手技能，以发现有价值的规律，并做出新的科学发现或工程创新。

四、课程教学方法

课堂讲授：人工智能基础知识主要通过课堂讲授。从人工智能的历史背景入手，介绍机器学习的基本概念和原理，着重讲解深度学习的基本原理和经典模型架构。此外，从科学与工程学的应用需求出发，介绍深度学习技术的优势和局限性，为后面的案例教学与实践训练打下知识基础。

案例教学：由生命科学、物质科学等领域的专家介绍科学问题和数据特征等 AI for Science and Engineering 应用场景，以及为何需要人工智能技术。之后，通过讲述实战成功案例，与

学生一起讨论分析人工智能如何帮助解决科研中的问题，引导学生思考如何理论联系实际，为实践训练项目作示范。

实践教学：主要通过习题课（tutorial）和课程实践项目（course practical project）两种形式，循序渐进地培养学生的动手实践能力。习题课帮助学生巩固在课堂学到的基本概念和理论知识，讲解作业难点，由助教示范和引导学生动手试验初步训练动手能力。在实践项目中，学生在领域专家和指导老师的引导下，从科学与工程中的实际场景中提炼出人工智能计算问题，通过数据处理、AI 模型构建与训练、测试和分析等一系列步骤，体验人工智能与数据科学项目的完整操作流程。

五、课程教学内容与安排

本课程教学内容分为三个模块：

（1）第 1 - 4 周：人工智能基础;

（2）第 5 - 8 周：AI for Science 案例研究;

（3）第 9 - 16 周：通过研究项目进行实践练习。

实践教学安排：

上半学期（第 1–8 周）主要以习题课（tutorial）的形式，内容包括助教回顾课堂讲授的重要知识点、讲解作业难点、示范 AI 建模解决问题等环节。学生在助教的指引下，动手实践，包括 Python 代码编写、模型构建和调试参数等。

下半学期（第 9–16 周）以课程实践项目的形式开展。学生们以 2-3 人组队的形式，在任课老师和助教的指导下完成整个数据科学全周期流程，包括文献调研，数据处理，AI 模型构建、训练、测试和分析等步骤。每周以组会的形式，由各个小组向指导老师汇报项目进展，然后讨论项目难点、

不足和改进方案，以研讨的方式培养学生批判性和创新性的思维和科研能力。最终写成项目报告，在期末做演讲汇报（Course Project Presentation）。

教学周	教学内容（主要知识点）	学时安排	教学方法
第一周	1. 课程概述：人工智能历史、任课教师介绍、评价规则等 2. 机器学习概述	4	课堂讲授
第二周	1. Python 测试 2. 深度学习的基础知识：介绍人工神经网络，训练深度神经网络等。	4	课堂讲授和习题课
第三周	深度学习的经典主题：卷积神经网络(CNN)、循环神经网络(RNN)、自编码器(Autoencoder)、图神经网络(GNN)等。	4	课堂讲授和习题课
第四周	人工智能前沿选题：Transformer、大型语言模型、生成式 AI、可解释人工智能等。	4	课堂讲授和习题课
第五周	人工智能赋能生命科学研究的案例教学	4	课堂讲授和习题课
第六周	人工智能赋能生命科学研究的案例教学	4	课堂讲授和习题课
第七周	人工智能赋能物质科学研究的案例教学	4	课堂讲授和习题课
第八周	人工智能赋能物质科学研究的案例教学	4	课堂讲授和习题课
第九周	课程实践项目	4	实践训练
第十周	课程实践项目	4	实践训练
第十一周	课程实践项目	4	实践训练
第十二周	项目中期汇报	4	实践训练
第十三周	课程实践项目	4	实践训练
第十四周	课程实践项目	4	实践训练
第十五周	课程实践项目	4	实践训练
第十六周	项目期末答辩和提交书面报告（具体时间和地点另行通知）	4	实践训练

六、考核方式和成绩评定方法

考核方式和具体占比：

（1）Python 测试：10%；

（2）随堂小测验和考勤率：10%；

（3）作业：30%（个人单独完成，总共三次作业，每次占 10%）；

（4）课程实践项目：50%（2-3 人组成一队，将在开学后专门发布评价标准，包括中期报告和项目最终报告的完成度、写作质量、方法的正确性和创新性，期末答辩表现等）。

其它相关规则：

（1）作业或报告迟交：截止时间之后 24 小时内提交答案或报告文件，评分扣掉 50%；迟交超过 24 小时，评分为 0。

（2）缺考、讲座或习题课缺勤或缺席项目汇报：如果没有正当理由且提前请假，将扣掉对应部分的分数。

七、教材和参考书目

	教材名称	教材作者	教材译者	ISBN	教材出版社	出版日期	教材版次
参考书目	Deep Learning for the Life Sciences	Bharath Ramsundar, Peter Eastman, Patrick Walters, Vijay Pande	N.A.	9781492039839	O'Reilly Media, Inc.	2019-05	第一版
	Deep Learning	Ian Goodfellow, Yoshua Bengio,	N.A.	9780262035613	The MIT Press	2016-11	第一版

		Aaron Courville					
	Deep Learning in Science	Pierre Baldi	N.A.	9781108955652	Cambridge University Press	2021-04	第一版

	教材名称	教材作者	教材译者	ISBN	教材出版社	出版日期	教材版次
推荐教材	Hands-On Machine Learning with Scikit-Learn, Keras & TensorFlow	Aurélien Géron	N.A.	9781492032649	O'Reilly	2019-10	第二版

八、学术诚信教育

本课程高度重视学术诚信，严禁抄袭、作弊等行为。“在学习、科研、实习实践等活动中，学生应恪守学术道德，坚守学术诚信，保护知识产权，坚持勇于创新、求真务实的科学精神，努力培养自己严谨求实、诚实自律、真诚协作的科学态度，成为良好学术风气的维护者、严谨治学的力行者、优良学术道德的传承者。”（具体请参见《上海科技大学学生学术诚信规范与管理办法（试行）》文件要求） 除非特别注明，否则您提交的作业应完全由您自己完成，并反映您的独立能力。 不要作弊: （1）不能抄袭他人答案的任何部分：助教和任课老师将自动和手动查重。 （2）不可以让其他人（无论是校内还是校外）代你做作业或项目。（3）在任何情况下，不要向其他学生展示、解释或分享你的作业；不要向小组队友之外的同学展示或分享你的项目报告和代码等相关资料。如果发生抄袭，被抄袭的学生将受到与抄袭他人的学生同样严厉的处罚。 （4）如果你的答案或报告中的某些句子来自书籍、论文或网络（例如维基百科），请注明参考来源并添加双引号，否则将被视为抄袭。 （5）如果你的项目解决方案中的一段源代码是从网络（例如 GitHub，ChatGPT）借用或改编的，你应该在代码和/或文档的注释中清楚地说明你是如何借用代码的。 （6）不违反学术诚信规则进行测验和考试（进一步的具体指示将在适当的时候给出）。 作弊后果：课程部分 0 分；不及格；在信用系统中留下记录；被大学开除。 对可再现性（reproducibility）的要求: （1） 你提交的解决方案应该能够被自己和他人独立地复现。 （2） 你的代码应该能够被再次运行，并且

其输出结果必须与你所报告的一致。 （3） 假如你的答案不可被再现，这将被判为“造假”，而得 0 分。

九、其他说明（可选）

无

AI for Science and Engineering Syllabus

1. Basic Course Information

Course Name	AI for Science and Engineering	Course Code	CS286
Course Level	undergraduate/graduate	Credit/Contact Hour	4/64
Major	Information science, life science, physical science, etc.	Teaching Language:	Bilingualism
Prerequisite		Prerequisite suggestion:	Python programming, probability theory and statistics, calculus, linear algebra
School/Institute	School of Information Science and Technology	Instructor	郑杰

*Notes: *Course level includes undergraduate, graduate, or undergraduate/graduate.*

***If multiple instructors are involved，please list the name of team leader.*

2. Course Introduction

Recently, artificial intelligence (AI) techniques have become more important in the research of science and engineering, partly because of the availability of large amounts of scientific data as well as the rapid advances and wide applications of deep learning methods. The main objective of this course is to enable students of different academic backgrounds to understand and use AI techniques in research projects. In the lectures, after introducing fundamentals of AI methods (especially deep learning), example applications of AI to scientific and engineering fields, including but not limited to material science, molecular biology, protein engineering, drug discovery, etc., will be described and

explained. Through hands-on exercises in tutorials, homework and course projects, students will be able to solve specific research problems using the state-of-the-art AI techniques. Furthermore, students will be able to develop novel AI techniques to push forward frontiers in science and engineering.

This course is characterized by project-based learning, which emphasizes the development of hands-on skills and linking theoretical knowledge with practical application closely. Therefore, of the 4 credits in this course, 2 are for theoretical learning and the other 2 for practical training.

3. Learning Goal

Cognitive competence: By taking this course, the students should be able to:

(1) Understand basic ideas of machine learning (especially deep learning) and other techniques of AI;

(2) Obtain experiences of solving scientific or engineering problems using AI techniques;

(3) Identify research problems that can be solved using AI techniques

(4) Select the most suitable machine learning methods for given research problems

(5) Propose innovations to improve the performance of existing machine learning methods, in terms of accuracy, computational efficiency, etc.

Comprehensive qualities: This is a research-oriented interdisciplinary course. Hence, by taking this course the students will be able to:

(1) Enhance their communication skills in collaborating with fellow students and researchers from different backgrounds;

(2) Building skills of creative and synthetic thinking to integrate knowledge and resources from different sources to solve a problem;

(3) Get or enhance hands-on skills of using computer software to explore multimodal data in order to find valuable patterns and make novel scientific discoveries or engineering innovations.

4. Textbook & Recommended Reading

	Book Title	Author	Translator	ISBN	Pubulisher	Pubulished Date	Edition
Textbook	Deep Learning for the Life Sciences	Bharath Ramsundar, Peter Eastman, Patrick Walters, Vijay Pande		9781492039839	O'Reilly Media, Inc.	2019-05	1st Edition
	Deep Learning	Ian Goodfellow, Yoshua Bengio, Aaron Courville		9780262035613	The MIT Press	2016-11	1st Edition
	Deep Learning in Science	Pierre Baldi		9781108955652	Cambridge University Press	2021-04	1st Edition
Recommended Reading	**Book Title**	**Author**	**Translator**	**ISBN**	**Pubulisher**	**Pubulished Date**	**Edition**
	Hands-On Machine Learning with Scikit-Learn, Keras & TensorFlow	Aurélien Géron		9781492032649	O'Reilly	2019-10	2nd Edition

5.Grading Policy

Evaluation methods and score proportion of the coursework components:

(1) Python test: 10%;

(2) Quizzes and attendance: 10%;

(3) Homework assignments: 30% (individual-based, a total of three assignments, each constituting 10%);

(4) Course practical project: 50% (in a team of 2-3 members; scoring scheme will be released after the semester begins, including the degree of completion of a project and the quality of writing as reflected in the interim report and the final report, the correctness and innovation of the method, and the performance in the final presentation, etc.

Other rules:

(1) Late submission of homework or project reports: If the homework or report is submitted within 24 hours after the deadline, 50% of the grade will be deducted; if it is submitted over 24 hours after the deadline, the score will be 0.

(2) Missing test, absence from lecture or tutorial, or absence from project presentation: If there is no valid reason and applying for leave in advance, the corresponding part of the score will be 0.

6. Instructional Pedagogy

Our instructional pedagogy is focused on project-based learning that links theoretical knowledge with hands-on skills for solving real-world problems in Science and Engineering.

Lectures: The basic knowledge of artificial intelligence is mainly taught in class. Starting from the historical background of artificial intelligence, this paper introduces the basic concepts and principles of machine learning, focusing on the basic principles and classical model architecture of deep learning. In addition, starting from the application needs of science and engineering, the advantages and limitations of deep learning technology are introduced to lay a knowledge foundation for the following case teaching and practical training.

Case study-based teaching: Experts in research fields (such as life science, material science etc.) will introduce specific application domains of AI for Science and Engineering, such as the scientific problems and data, and why AI technology is needed. After that, by telling success stories of AI, the

lecturers will discuss and analyze with students about how AI can help solve the problems in scientific research. Such case studies can guide the students to think about how to link theory with practice, as a preparation for their practical training projects.

Practical training: Mainly through two forms of practical training, i.e. tutorial and course practical project, this course will cultivate students' hands-on practical skills step by step. First, in the tutorials, Teaching Assistants (TAs) will help students enhance their understanding of the basic concepts and theoretical knowledge learned in the lectures, explain some key points in homework assignments. Moreover, the TAs will demonstrate and guide the students to conduct hands-on experiments to train their hands-on skills. Secondly, in the practical project, under the guidance of instructors who are also scientific domain experts, students learn how to transform real-world challenges in Science and Engineering into computational problems to be tackled by AI, and go through the whole life-cycle of AI and data science projects, including a series of steps such as data processing, AI model construction, training, testing and analysis, etc.

7. Course Structure

The teaching contents of this course can be divided into 3 modules:

(1) Weeks 1 – 4: Foundations of AI;

(2) Weeks 5 – 8: Case studies of AI for Science and Engineering;

(3) Weeks 9 – 16: Hands-on training by working on course practical projects.

Arrangement of practical training:

In the first half of the semester (weeks 1-8), the training is mainly in the form of tutorials, during which TAs help students review key points of knowledge taught in the lectures, explain difficult parts of the homework, and demonstrate how to build AI models to solve problems, etc. Under the guidance of the TAs, students will do hands-on work, including Python coding, model building, and parameter tuning, etc.

In the second half of the semester (Weeks 9-16), the training takes the form of course practical project. Students work in teams each of 2-3 members, under the guidance of professors and TAs to complete a complete life cycle of a typical data science project, including literature survey, data processing, AI

model construction, training, testing and analysis. In the form of weekly group meeting, each group presents the progress of project to the instructors and then they discuss together the challenges, limitations and improvement plans of the project. Such group meetings can cultivate students' critical and innovative thinking as well as scientific research ability. Finally, to communicate their research, the students are required to write project final reports and give presentations on their work.

Week	**Teaching Contents**	**Contact Hours**	**Teaching Modes**
Week 1	1. Overview of course (history of AI, instructors, evaluation, etc.) 2. Overview of machine learning	4	Lecture
Week 2	1. Python test 2. Basics of deep learning: Introduction to artificial neural networks, training deep neural networks, etc.	4	Lecture & Tutorial
Week 3	Classic topics of deep learning: Convolutional neural networks (CNNs), recurrent neural networks (RNNs), autoencoders, graph neural network, etc.	4	Lecture & Tutorial
Week 4	Selected topics of AI: Transformer, large language models, generative AI, explainable AI, etc.	4	Lecture & Tutorial
Week 5	Case studies of AI in Life Sciences	4	Lecture & Tutorial
Week 6	Case studies of AI in Life Sciences	4	Lecture & Tutorial
Week 7	Case studies of AI in Physical Sciences	4	Lecture & Tutorial
Week 8	Case studies of AI in Physical Sciences	4	Lecture & Tutorial
Week 9	Learning by working on projects	4	Practical training
Week 10	Learning by working on projects	4	Practical training
Week 11	Learning by working on projects	4	Practical training

Week 12	Mid-term presentations by students	4	Practical training
Week 13	Learning by working on projects	4	Practical training
Week 14	Learning by working on projects	4	Practical training
Week 15	Learning by working on projects	4	Practical training
Week 16	Project presentations by students (specific time and venue to be announced)	4	Practical training

8. Academic Integrity

This course highly values academic integrity. Behaviors such as plagiarism and cheating are strictly prohibited. Unless explicitly noted, your work submitted should be done all by yourself and reflect your independent capabilities. Please do not cheat: (1) No plagiarism (i.e. copy any part of solution from others): We will scan your solutions for similarity both automatically and manually. (2) Do not ask anyone else (whether inside or outside the university) to do the homework or project on your behalf. (3) Do not show, explain or share your homework or project solutions to (with) any other student under any circumstance. In case of plagiarism, a student being copied shall be punished as severely as a student copying others. (4) If some sentences in your answer or report are from books, papers or web (e.g. Wikipedia), cite the sources as references and add double quotations. Otherwise, it is counted as plagiarism. (5) If a piece of source code in your project solution is borrowed or adapted from the web (e.g. GitHub), you should state clearly as comments in the code and/or in document how you have borrowed the code. (6) Do not violate academic integrity rules for quizzes and exam (further specific instructions will be given in due time). Consequences of cheating: 0 score for course component; fail the course; record in credit system; expulsion from the university. Reproducibility is required: (1) Solutions you submit should be reproducible independently by yourself as well as others. (2) Your program is expected to run again to output results consistent with you report. (3) An answer not reproducible is considered a “fake solution”, and will get 0 score.

N.A.

9. Other Information (Optional)