GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	R language in chemistry: data analysis and visualization, PG_00069260		
Field of study	Chemistry		
Date of commencement of studies	February 2025	Academic year of realisation of subject	2025/2026
Education level	second-cycle studies	Subject group	
Mode of study	Full-time studies	Mode of delivery	at the university
Year of study	1	Language of instruction	Polish
Semester of study	2	ECTS credits	3.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Department of Physical Chemistry -> Faculty of Chemistry -> Wydziały Politechniki Gdańskiej		
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. inż. Adam Kloskowski	
	Teachers		

Lesson types and methods of instruction

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	0.0	0.0	45.0	0.0	0.0	45

E-learning hours included: 0.0

Learning activity and number of study hours

Learning activity	Participation in didactic classes included in study plan	Participation in consultation hours	Self-study	SUM
Number of study hours	45	5.0	25.0	75

Subject objectives

The aim of the course is to introduce students to the practical possibilities of using artificial intelligence (AI)-based tools in chemical sciences. The course is of an applied nature and focuses on the effective, critical and responsible use of modern AI tools - such as ChatGPT, Perplexity AI, Elicit, SciSpace, ResearchRabbit, etc. - for planning experiments, supporting data analysis processes, developing documentation and automating repetitive tasks. After completing the course, the student should: 1) know and understand the basic principles of generative AI and large language models (LLM), 2) be able to formulate effective queries (prompts) tailored to a specific research problem to obtain valuable and accurate answers, 3) be able to effectively use selected AI tools such as ChatGPT, Perplexity AI, Elicit, SciSpace, ResearchRabbit to support scientific work in chemistry or related sciences, 4) be able to create AI agents and organize their work into a team of AI agents to perform repetitive tasks (e.g. data collection, preliminary data control, data analysis and visualization, report generation, etc.), 5) be aware of the risks associated with AI hallucinations and know the methods to limit this phenomenon, 6) know the basic principles of ethical and safe use of AI.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[K7_U04] develops and transmits technical information in the form of text documents, spreadsheets, graphs, technological diagrams and multimedia presentations, and prepares a speech including a multimedia presentation	The student prepares and conveys technical information in the form of text documents, spreadsheets, graphs, technological diagrams and multimedia presentations, and prepares a speech including a multimedia presentation	[SU1] Assessment of task fulfilment [SU3] Assessment of ability to use knowledge gained from the subject
[K7_W01] recognizes problems of modern chemistry, including properties and obtaining chemical compounds, necessary for making calculations, including the dependence of the compound's structure and its reactivity	The student recognizes the problems of modern chemistry, including the properties and preparation of chemical compounds, necessary to perform calculations, including the dependence of the compound's structure and its reactivity	[SW1] Assessment of factual knowledge
[K7_K02] is able to cooperate and work in a group, taking on different roles	The student is able to cooperate and work in a group, assuming different roles in it.	[SK1] Assessment of group work skills [SK2] Assessment of progress of work

Subject contents	The content covered in the lecture covers the following areas: 1) Concepts and introduction to generative AI and large language models (LLM) - architecture, mechanisms of action and application of language models such as ChatGPT, LLaMA, Claude or Gemini in the context of chemical and natural sciences. 2) Prompt engineering - principles of effective prompting, query formulation techniques, the role of context, structure and precision in obtaining accurate answers. 3) AI hallucinations and credibility of generated information - mechanisms of errors in generated content, methods of recognizing them and minimizing their impact (quality of training data, contextualization of prompts, fact checking). 4) Principles of ethical and safe use of AI in chemical sciences: user responsibility, source transparency, copyright and limits of AI use in scientific work. 5) Creating AI agents and AI agent teams: theoretical foundations of building AI agents, their tasks and cooperation within multi-agent systems to automate repetitive activities. 6) The future of AI in chemical sciences: directions of development, examples of AI tools (ChatGPT, Perplexity AI, Elicit, SciSpace, ResearchRabbit), examples of AI use in chemistry and related sciences, e.g. for analyzing HPLC results, spectroscopy, experimental statistics, etc. The content discussed in the lab covers the following areas: 1) Overview of the most popular language models ChatGPT, LLaMA, Claude, Gemini, etc., 2) Creating effective prompts - practice of writing scientific, technical and analytical queries and their modification for better results, 3) Practical introduction to designing AI agents and AI agent teams for specific tasks - Defining OKRs (Objectives and Key Results), lists of rules, personalities, selection of temperature/level of creativity, etc., 4) Analysis and visualization of research results using AI - generating graphs, tables, infographics for presenting results, 5) Case study - solving a real research problem using AI (from concept to final report). Individual or team work using various AI tools.
Prerequisites and co-requisites	

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
	60.0%	50.0%
	50.0%	50.0%

Recommended reading	Basic literature	Andrzej Kacprzak. Prompt engineering i ChatGPT. Poradnik skutecznej komunikacji ze sztuczną inteligencją. Wydawnictwo: ISBN: 978-83-289-1362-2. Olivier Caelen, Marie-Alice Blete. Tworzenie aplikacji z wykorzystaniem GPT-4 i ChatGPT. Buduj inteligentne chatboty, generatory treści i fascynujące projekty. Helion 2024, ISBN: 978-83-289-1044-7.
	Supplementary literature	James Phoenix Taylor Mike. Skuteczna inżynieria promptów. Przyszłościowe rozwiązania dla rzetelnych wyników generatywnej AI. Helion 2025, ISBN: 978-83-289-1904-4.
	eResources addresses	

Example issues/ example questions/ tasks being completed	Example theoretical topics: - What is generative AI and how does it differ from traditional AI? - Explain the transformer architecture as the basis for the operation of large language models. - What are the basic differences between ChatGPT, Claude, and Gemini models? - How does the process of "training" a large language model work? - List and characterize examples of LLM applications in chemistry. - What is tokenization in language models? - What does the concept of "prompt engineering" mean and why is it important in working with AI? - What elements should an effective scientific prompt contain? - Explain what "Zero-Shot", "One-Shot", and "Few-Shot Prompting" are. - Present the difference between open, closed, and contextual prompts. - How to formulate a prompt for AI to obtain a summary of scientific literature? - Why is it important to provide context in prompts? - What is "prompt leakage" and how does it affect the AI-generated response? - Propose a prompt for analyzing HPLC results using ChatGPT. - What are so-called AI hallucinations and why are they problematic in scientific work? - What factors increase the risk of hallucinations in AI-generated responses? - How can you recognize an unreliable language model response? - Discuss the role of training data quality in the context of AI hallucinations. - What tools or techniques can support fact-checking of AI-generated information? - How can you assign a personality and communication style to an AI agent? - How are the goals and principles of action for a single AI agent defined?
Work placement	Not applicable

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