

ChatGPT: Application in Chemistry Education and Challenges

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Abstract

The paper discusses the advancements and applications of neural networks, specifically ChatGPT, in various fields, including chemistry education and research. It examines the benefits of AI and ChatGPT, such as their ability to process and analyze large amounts of data, create personalized training systems, and offer problem-solving recommendations. The paper delves into practical applications, showcasing how ChatGPT can be utilised to augment chemistry learning. It provides examples of using ChatGPT for creating tests, generating multiple-choice questions, and studying chemistry in general. Concerns are voiced about the ethical and societal impact of AI development. In conclusion, it explores the exciting potential of AI to tackle challenges that may exceed human capabilities alone, paving the way for further exploration and collaboration between humans and intelligent machines.

Keywords

ChatGPT 3.5, Artificial Intelligence, AI for Education, Computer-Based Learning

1. Introduction

A neural network is an attempt to represent a particular phenomenon as a very cumbersome, multidimensional but simple and understandable system—a network. It is an example of the artificial intelligence, AI, implementation. At the same time, it is necessary to prove that multidimensional linearization can replace reality. The question arises: why do this? Is it to know the truth? Is it to obtain, at least, an approximate but truthfully close interpretation and understanding? In essence, the problem boils down to finding a black cat in a dark room. It remains unclear whether it is there, whether we need to look for it, and

whether it will transform into a tiger while we search.

Currently, neural networks and AI developments are increasingly being used in various fields, including education and research. Using these technologies, one can solve problems related to data processing and analysis, process automation, as well as the creation of personalized training systems and decision support tools [1] [2].

The widely used ChatGPT neural network is a language model developed by OpenAI based on the GPT (Generative Pre-trained Transformer) architecture for understanding and writing text. The operation of ChatGPT is based on the use of pre-existing textual data. Its application covers various fields including content creation, translation, code generation [3], it can also be used for educational purposes [4] [5].

Thus, it can help by simplifying complexly written text, provide examples for clarity, and offer problem solving recommendations. Teachers can use ChatGPT to create teaching materials, or even simulate discussions for educational purposes, further expanding the technology's educational capabilities [6] [7].

However, like any technological advancement, ChatGPT is not without its challenges. Thus, there are issues related to bias, misinformation propagation, and the model's susceptibility to generating inappropriate or harmful content [8] [9]. Other problems include privacy and data security issues, as well as transparency and explainability [10]. Understanding and addressing these challenges is crucial for optimising the performance and ethical implications of ChatGPT.

Artificial intelligence is highly anticipated to play a key role in developing control systems with significant uncertainties. Neural networks are proposed to address the challenge of lacking accurate mathematical models for various processes, encompassing social, chemical, and physical domains. However, studies conducted by the authors on technical systems with inherent uncertainties and nonlinearities raise a crucial point: inaccuracies within neural networks and their corresponding models can lead to significant issues in AI-powered systems [11] [12] [13] [14]. The very nature of neural networks adapting their structure to the controlled objects poses a significant challenge in achieving desired compensation and controllability. The theoretical basis for these problems is the theory of systems with variable parameters [15] [16].

2. Advances in the Application of Neural Networks

Recent success in the application of neural networks is undeniable. Unmanned driving, technical vision, automatic translations, big data, personalised medicine, compiled texts, music, images, etc. are all undeniable advances associated with a very powerful leap in electronics and software. In fact, we are creating the universal soul of nature that Chekhov mentioned in "The Seagull" [17]. True, he did not reveal its details: the author of the idea ends his life at the end of the play. Is there nothing to fear for mankind now, after 120 years? It may be logical that a human being cannot bear such a burden. And the World Wide Web? At least to

accumulate data, which, perhaps, only a higher being can comprehend.

Have we been overcome by pride again? The Tower of Babel also comes to mind: its construction began with a single language. However, maybe our task is simpler after all?

Almost until the end of the 20th century, chess was considered the standard of human intelligence, and its algorithms were unattainable for automatic machines. However, in the 21st century, a simple computer is able to play at the strength of a master without any mysticism [18]. Still, a computer cannot create a game like chess, although attempts to develop games with the help of AI are already underway. For example, in 2023, programmers from Luden.io [19] developed the game "Generated Adventure" [20] in just 72 hours using AI technologies.

Obviously, no person or group of people can compete with ChatGPT in terms of memory capacity and instantly find the answer to any question. In addition, humanity has reached dead ends from which neither politicians nor philosophers see a way out, and AI can help to resolve some issues [21].

The benefits of AI and ChatGPT, in particular, are beyond question. Now, ChatGPT is a vast reference book or a "world soul," according to Chekhov, which remembers everything but does not exist. Humanity needs it. Therefore, it will be created—there is no doubt about it. And it will be improved. The fact that Chekhov's character committed suicide at the end of the play will not stop anyone. Nobody knows where that ending is.

3. Experimental

3.1. ChatGPT Application

3.1.1. For Creating Tests

Let's look at some options for using ChatGPT for teaching and research in the field of chemistry. As part of this work, ChatGPT 3.5 was used to generate incorrect answers to questions for analytical chemistry tests. That is, the questions were compiled using the provided educational materials, and the incorrect answers were generated using a neural network.

User: "Write three incorrect answers to the question: 'What is the precipitation titration curve of a mixture?' for Chemistry test and mark them as 1), 2) and 3)".

ChatGPT 3.5:

"1) The precipitation titration curve of a mixture is a graph illustrating the changes in temperature during the titration process, indicating the ideal conditions for precipitation.

2) It is a visual representation of the chemical composition of a mixture before and after the precipitation reaction, demonstrating the elements involved and their concentrations.

3) The precipitation titration curve displays the different stages of a mixture turning into a solid, showing the time it takes for complete precipitation to oc-

cur".

The suggested answers were suitable for the test. This use of ChatGPT significantly speeds up the test creation process.

Furthermore, the following option was tested: a text was uploaded to ChatGPT to test the neural network ability to generate multiple-choice questions. Most of them were suitable for inclusion in the test.

3.1.2. For Studying Chemistry

Sometimes students need to quickly answer questions on a subject that interests them. While ChatGPT can be consulted, its answers may not always be correct [22], therefore, clear queries are essential. As an experiment, ChatGPT 3.5 was asked questions from the field of organic, analytical chemistry and physico-chemical research methods, discussed below.

Organic Chemistry question: "Is the reaction between toluene and srearic acid possible?"

ChatGPT 3.5: "The reaction between toluene and stearic acid typically involves Friedel-Crafts acylation, where toluene reacts with stearic acid in the presence of a Lewis acid catalyst, such as aluminum chloride. This can lead to the formation of an acylated product. Keep in mind that reaction conditions and specific reagents can vary based on the desired outcome".

Analytical Chemistry Question: "What happens when you mix two different buffer solutions?"

ChatGPT 3.5: "The resulting solution will likely have a different pH than the original buffer solutions. The pH of the resulting solution will depend on the specific components and concentrations of the buffers being mixed. Buffers are designed to resist changes in pH, but when you mix them, the combined buffer-ing capacity may change, affecting the overall pH of the solution".

A question on physicochemical methods of analysis: "In many cases, when doing IR spectroscopy, a tablet is prepared with potassium bromide. Why is this preferred over simply making a tablet from just the test substance?"

ChatGPT 3.5: "While it might be possible to make a pill directly from the test substance, using KBr offers several advantages in terms of consistency, transparency, and ease of handling. KBr is relatively inert and does not strongly interact with most substances. This helps prevent any unwanted chemical reactions or interactions that could affect the analysis. Additionally, some substances might not form suitable pellets on their own, and using KBr helps overcome these challenges. It's worth noting that the choice of sample preparation method can depend on the nature of the sample and the specific requirements of the analysis".

It is obvious that ChatGPT, based on the information it provides, gives correct and clear answers, *i.e.* it makes sense to use it for quick information retrieval when studying chemistry. To control the size of the article, here are shortened ChatGPT answers. Sometimes, if one need a more detailed answer or clarification of some points of the received answer, it is necessary to ask ChatGPT additional questions.

In scientific work, it is occasionally necessary to publish articles on ready-made material or to apply for a patent. Usually there is some scientific background, but the writing style of each researcher is special. To avoid similarities with their own work, it is convenient to use ChatGPT for paraphrasing [23] [24].

While ChatGPT shows a significant decrease in plagiarism occurrence in texts, it's important to highlight that the current level of plagiarism is still relatively elevated (45%) and is considered unacceptable by many academic journals [25].

3.1.3. For Scientific Assumptions

ChatGPT was used to generate ideas for writing intermediate conclusions on a highly specialised work. Let us consider an example from the field of organometallic chemistry and chemistry of coordination compounds.

The research objects are triarylantimony complexes with oximate or carboxylate ligands. The molecules have a similar geometry of the central metal atom. It can be explained using Valence Shell Electron Pair Repulsion (VSEPR) theory [26]. This theory posits that electron pairs in the valence shell of an atom repel each other and will therefore arrange themselves in a way that minimizes this repulsion, leading to specific molecular shapes. Some differences in the molecular structures were found, and ChatGPT offered the reason for them.

User: "Triarylantimony dioximates are molecules with trigonal bipyramidal coordination. According to the VSEPR theory and Gillespie assumption, in the molecules with trigonal bipyramidal coordination of the central atom, the equatorial bonds are shorter than the axial ones. This is true, for example, for triarylantimony dicarboxylates. Explain why the situation is different for triarylantimony dioximates, where axial bonds are shorter than the equatorial ones? The aryl groups in triarylantimony dioximates are the same as in triarylantimony di-carboxylates".

ChatGPT 3.5: "The presence of different ligands or substituents can alter the electronic structure of the molecule. In triarylantimony dioximates, the dioximate ligands introduce additional electron density around the central antimony atom. This alteration in the electronic structure can impact the distribution of electron pairs and influence bond lengths.

The coordination preferences of dioximate ligands may differ from dicarboxylate ligands. The specific nature of metal-ligand interactions, including any potential pi-bonding or other coordination effects, can influence bond lengths differently in dioximates compared to dicarboxylates".

User: "Why there is the additional electron density around the central antimony atom in triarylantimony dioximates compared to triarylantimony dicarboxylates?"

ChatGPT 3.5: "The additional electron density around the central antimony atom in triarylantimony dioximates compared to triarylantimony dicarboxylates is a consequence of the nitrogen lone pairs in the dioximate ligands, which have a higher electron-donating ability compared to the oxygen atoms in dicarboxylate ligands. This difference in ligand electronic properties influences the overall electronic structure of the coordination complex".

After a clarifying question, the answer becomes clear: oximate ligands possess a greater ability to donate electrons than carboxylate ligands, which plays a role in shaping the electronic structure of the coordination complex. Therefore, obviously, ChatGPT is able to make assumptions based on the theory loaded into it. Although there are no answers to these particular questions, it is able to find similar information in the available sources to answer these questions.

3.2. Challenges

3.2.1. About Paradoxes

Consider a more creative approach to problem solving. How can ChatGPT find solutions to questions that do not currently have answers (or even similar questions)? It is unlikely that this can be accomplished by a continuous search of connections. Still, it is necessary to formulate the principle of searching for paradoxes and ingenious solutions according to some not very clear criteria. But there is hope that with knowledge and time these unclear paths will be clarified.

What pushes thoughts onto one path or another, which at first does not at all resemble a solution? It is not clear yet. Maybe, after all, brute force is the only way, false moves are erased from memory and it seems that the solution was direct and logical. It is difficult to formulate a solution algorithm; the paths for its movement are accessible to few people. The purpose of the experiment is to find out whether, using ChatGPT 3.5, it is possible to find an answer to a question that people could not answer and which cannot be found in the memory of the "world soul".

User: "Do you know Euclid's 5th postulate?"

ChatGPT 3.5: "Yes, Euclid's Fifth Postulate is also known as the Parallel Postulate, and it is one of the five postulates in Euclidean geometry."

User: "Can you prove it?"

ChatGPT 3.5: "The Parallel Postulate has a long history of attempts to prove it or derive it from the other postulates. However, it was eventually discovered that the Parallel Postulate is independent of the other postulates and cannot be proven or derived from them."

User: "Is it necessary to prove Euclid's 5th postulate?"

ChatGPT 3.5: "While it might not be necessary in the practical sense, as Euclidean geometry itself is highly useful and applicable, the exploration of the Fifth Postulate and its implications contributed to the broader understanding of mathematical systems and the nature of geometry. It highlighted the idea that different sets of axioms could lead to internally consistent yet distinct mathematical structures."

User: "What consequences will there be if the evidence is found?"

ChatGPT 3.5: "Discovering a proof of Euclid's Fifth Postulate from other postulates would impact the self-contained nature of Euclidean geometry, influ-

ence foundational quests in mathematics, deepen our understanding of alternative geometries, provide insights into historical challenges, and potentially lead to adjustments in educational curricula. The independence of the Parallel Postulate remains a fundamental aspect of the foundations of geometry. The discovery of such evidence would represent a significant development in the history and philosophy of mathematics."

In this experiment, it does not matter at all whether this is a complete answer. It is important how ChatGPT responds, particularly whether it seeks out novel connections and reasoning not yet discovered. Faced with a question where no answer exists in its memory, ChatGPT doesn't simply stop. Instead, it identifies the closest match from its known options. Essentially, this is its operating principle. In its own words, ChatGPT answers questions using its training data, which includes a diverse range of sources from the internet. It understands context and can generate responses based on the patterns and information it has learned during training.

Does this non-learning algorithm guarantee its controllability, and is it the only option when faced with questions challenging traditional logic, like paradoxes? As ChatGPT 3.5 itself states, it does not have the ability to self-learn or update its knowledge over time. This is a static model that was trained on a diverse range of internet text up until its last training cut-off in January 2022. It does not have the capability to access new information or adapt to changes that occurred after this cut-off. Does this limitation compromise its controllability, and are there alternative approaches for tackling such complex questions?

Therefore, ChatGPT first finds the answer in memory, and then links it to the question. At first, it tries to match questions to its existing knowledge, but it can also generate creative responses or acknowledge when it doesn't have a clear answer. The question will come to a solution in any case. Is it possible to find the solution that does not exist?

3.2.2. The Relationship between Intuition and Resilience

Are neural networks capable of solving paradoxes? Are they taught this ability? While the study of intuition might face limitations and become concentrated among a few experts, this doesn't necessarily mean it becomes inaccessible. Researchers can develop algorithms to search for unstable solutions. With future computing power, finding a single relevant solution among billions might become possible, similar to advancements in AI chess playing.

We can be sure that the "Intuitive Search for Solutions" algorithm will reveal its mechanisms with time and knowledge. It is unlikely this algorithm will be based on something like a neural network, where search is the main focus of the algorithm. An AI system searching for an unknown solution should create controlled instability, similar to a genius who, in a way known only to them, finds an unexpected solution. Think of Archimedes guessing the Earth is round, Einstein unifying particles and waves, or a poet composing, "...the mountain peaks sleep in the darkness of the night..." [27]. Currently, ChatGPT does not try to find new unknown connections and solutions. A paradoxical solution is most likely an unstable process that has found unexpected intuitive connections and solutions. At the end of the chain there is an unexpectedly correct solution with a whole system of new connections. A neural network will be able to find such a solution if the initial signs and logic of intuitive movement are explained to it but there are no such prerequisites yet. A search based on selecting all possible connections is hardly possible. Is it possible to play chess with constantly changing rules?

Intuition will be explained and at the same time compressed. That is, AI will catch up with a person as a person gets to know themselves and transfers their knowledge to AI.

3.2.3. About Neural Networks in Management Risks

Despite their initial focus on mathematics and technology, neural networks haven't seen widespread application in areas like advanced control systems, where even basic regulators often rely on outdated and inefficient approaches with limited AI integration. Blindly relying on simplified models of complex systems for control can be dangerous. Therefore, control can be adapted to reality by compensating for the peculiarities of the object. According to the theory with variable parameters, this can only be done only by exactly replicating the object. Linearisation of reality will not work, it will lead to unpredictable consequences.

The fundamental work on the theory of systems with variable parameters [15] [16] considers a compensating technique for the variable inertia of dynamic structures by including sequentially forcing circuits, as demonstrated by Equations (1) and (2).

$$V_{1} = \left(a_{n}(t) \cdot p^{n} + \dots + a_{1}(t) \cdot p + a_{0}(t)\right).$$
(1)

$$V_{2} = a_{n}(t) \cdot p^{n} + \dots + a_{1}(t) \cdot p + a_{0}(t).$$
⁽²⁾

As Equation (3) shows, the variable operators should be strictly matching.

$$a_n(t) = a_n(t). \tag{3}$$

If the operators in the relaxation forcing circuit are all equal for all t, the chain turns into a link with a unity operator:

$$V_1 V_2 = 1$$
. (4)

That is, compensation occurs if only all variable parameters of the operators coincide at each point in time.

Equation (5) describes the effect of one variable operator on another:

$$V_{1}^{*} = \sum_{\lambda=0}^{m} \frac{d^{\lambda} V_{2}}{dp^{\lambda}} \cdot V_{1} \frac{p^{\lambda}}{\lambda!} = V_{1} \cdot V_{2} + \sum_{\lambda=1}^{m} \frac{d^{\lambda} V_{2}}{dp^{\lambda}} \cdot V_{1} \frac{p^{\lambda}}{\lambda!} .$$
 (5)

If the operators of the relaxation and forcing circuits do not coincide, except for the structure defined by Inequality (6),

$$\neq 1 = \frac{\sum_{0}^{n} a_{i}(t) p^{i}}{\sum_{0}^{n} a_{i}^{*}(t) p^{i}},$$
(6)

an equalizing operator with a very cumbersome and unpredictable transfer function (Equation (7)) appears.

$$\sum_{\lambda=1}^{m} \frac{d^{\lambda} V_2}{dp^{\lambda}} \cdot V_1 \frac{p^{\lambda}}{\lambda!}.$$
(7)

This operator is almost never taken into account in technical systems. Essentially, in systems with neural networks, there may be no complete correspondence between digital correction systems and real objects. This implies that during direct correction, equalizing operators, *i.e.*, unpredictable phenomena, will be inevitable.

If one tries to adapt to the changes in the world, but at the same time consider that the world develops according to the principles one has formed oneself and believe in, without paying attention to the reality, the result may be sad and certainly unexpected.

Sometimes, very rarely, there is luck, but is it worth counting on this rare luck? Any approximate solution can be quite effective in any particular case. It is important to understand this correct range and stop on time.

4. Conclusions

ChatGPT has shown promise in the field of chemistry. It is effective in tasks like creating tests and generating answer prompts for students. Additionally, it can be used to paraphrase scientific texts. Overall, ChatGPT can greatly facilitate the work of researchers and students associated with this field of science.

While ChatGPT excels at finding relevant information within existing data, it struggles to offer truly novel solutions to completely unknown questions. However, its ability to suggest possibilities based on similar answers can be helpful in scientific work. This approach needs further refinement to ensure the suggested answers are genuinely relevant and not just superficially related. When it comes to "unstable decisions" and complex challenges like paradoxes, it remains unclear whether neural networks like ChatGPT have the capacity to effectively navigate these scenarios. Further developments and exploration of capabilities of neural networks could prove their benefits in this field.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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