Ethical Note - Image Recognition of Chemical Molecules

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1 Introduction

The development and deployment of machine learning algorithms is of significant with respect to ethical responsibilities. Although our objective is to automate the analysis of reaction schemes, particularly in water treatment studies, we must consider with great importance the possible impacts on the integrity of research, data collection, transparency, and data privacy. This paper outlines key ethical questions related to this project and our approach to answering these questions.

2 Ethical Considerations

2.1 Data Collection

To ensure effectiveness and ethical integrity of our machine learning algorithm, we implemented a careful approach to data collection.

We prioritized the insertion of diverse and characteristic data to reflect various chemical formulas, arrow tips, and lines commonly found in scientific lectures. By gathering these datas into one single dataset, we created a dataset creation algorithm which positions different combinations of chemical formulas, arrow tips, and lines randomly placed in order to correctly train our algorithm.

While creating these datasets, we used publicly available scientific letters and publicly available data repositories in order to ethically create our dataset. This approach leads us to respect the authors that do not want to share or autorise to use their research in our respective one. These repositories are all comply with open source politics.

2.2 Transparency and Explainability

For machine learning algorithms like we create; transparency, interpretability and explainability are concepts that are closely related to data ethics and necessary to build trust in their safe usage[1].

For transparency, we made an effort to publish all of our codes, their explanations and if it is taken from another open-source code their origin in an open-source format to encourage external reviews and feedback.

Explainability holds significant importance, especially in critical applications such as healthcare[2]. By emphasizing explainable ML principles, our goal is to equip users with the necessary tools to interpret, assess, and confidently rely on the results produced by our model.

For improving the explainability of our code, instead of providing a result directly, we allow users to view the steps taken during the process—such as detecting arrows, backtracking to identify lines, and converting chemical formulas into their respective SMILES representations. Additionally, we have included detailed comments in every part of the code and provided a concise summary at the beginning of each file. This ensures that others can easily understand, use, and contribute to our project.

Additionally, we have committed to ensuring that explainability does not compromise model performance, as recent studies have shown that well-designed interpretable ML systems can maintain high accuracy while providing meaningful explanations[3].

2.3 Misuse of the Algorithm

While our algorithm's preliminary objective is satisfied, we must question the potential misuse scenarios of our algorithm.

There are serious concerns for the case where individuals put unknown molecules into our algorithm to examine how they change when they make contact with water. Because the resulting molecules and effects are unpredictable, these studies into unknown molecular interactions may produce unpredicted results. The primary worry is the uncertainty surrounding the transformation or breakdown of these unidentified compounds, which could produce chemicals with unknown effects.

To limit and minimize these risks, we planned to implement some key safety measures further down our project. We will restrict the access to use the algorithm to only authorized researches and institutes. We want to maintain transparency and explainability of our code through detailed documentation. Additionally, we will try to create a detection system to identify and restrict molecules outside confirmed safety parameters.

These measures ensure that our contributions to molecular recognition technology progress responsibly while upholding scientific integrity. Our approach harmonizes innovation with ethical principles, emphasizing societal benefit and safety.

References

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