A Mobile App for Exploring Chemical Molecules:

Machine Learning-Powered Handwritten Compound Identification and 3D Visualization

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Abstract—**The study of Chemistry is part of the mandatory school curriculum in Brazilian basic education and is considered by students to be a difficult subject to understand and abstract, generating resistance in learning, assimilation of concepts, and applicability in everyday life. As an experimental science, laboratory practice has contributed to students' learning. However, it is not always possible to carry out experiments, as many schools do not have the necessary physical requirements or for classes that are taught online. This article presents the development of a mobile application that uses machine learning to improve the process of teaching chemistry, making it possible to identify hand-drawn molecules and display 3D virtual correspondents, showing the structure of the element as well as information that relates it to everyday life.**

Keywords - Chemistry; education; machine learning; mobile app; CoreML.

I. INTRODUCTION

The important role that technological resources have played in our contemporary society is indisputable. Nowadays, mobile devices are widely used, facilitating all areas of daily life, and significantly evolving into practically inseparable extensions of our bodies and our minds. In this context, the crucial importance of integrating them into the teaching and learning process is highlighted, especially given that, in today's day and age, young students are born and grown in an intrinsically technological society [13].

However, despite the conveniences offered by a technological world, certain academic subjects, especially chemistry, remain a great challenge to many students. In the classroom setting, chemistry education often unfolds through static representations on chalkboards or whiteboards, where intricate molecular structures are sketched in abstract notations and symbols. While these methods serve as initial blueprints, they also pose a difficulty for students, given that it is inherently challenging to understand and comprehend a complex subject solely through static drawings and abstract concepts, added to the fact that they cannot see it in their daily lives or understand how it affects them [14].

This paper shows the development process of a mobile app aimed at helping students with the challenges of learning chemistry, with the integration of technology. It benefits their learning process, while also helping them identify drawn 2D static molecules presented to them in the classroom and understand the meaning and importance of it. By bridging this gap between abstract concepts and the real-world, the application aims to make the study of chemistry more accessible and engaging, offering an interactive alternative solution to understand the subject and appreciate the presence of these structures in their everyday lives.

The remaining of the paper is structured as follows. Section 2 presents how the use technology enhances chemistry education and addresses learning challenges. Section 3 presents the topic of supervised machine learning and CNNs to classify hand-drawn chemical molecules. Section 4 presents the development of an educational app for learning chemistry through machine learning-powered molecule recognition. Section 5 presents the developed application, an interactive app for identifying and learning about hand-drawn chemical molecules. Section 6 presents the possible empowerment of Brazilian education with a machine learning app for interactive chemistry learning.

II. CHEMISTRY EDUCATION AND VISUAL-BASED LEARNING

The challenges faced during the teaching and learning process often result in significant failure rates and a growing lack of interest on the part of both students, who face learning difficulties, and teachers, who feel challenged to impart knowledge [1]. This difficult challenge is particularly noticeable in the teaching of chemistry, which can be attributed to traditional methods that combined with complex content, make classes monotonous and discouraging.

The study of chemistry poses a challenge in visualizing molecule structures and their complexities, especially in settings where laboratories are scarce and access to visual aids and interactive learning is not guaranteed. In 2019, only 42,1% of public high schools in Brazil had Science laboratory structures, while, in public middle schools, that number got as low as 8,6% [7]. Furthermore, considering the Brazilian standardized high school exam (ENEM), which can be used to understand better students' performance on mandatory subjects, data shows that candidates performed below 50% in questions that include chemical equations and symbols (INEP, 2019), which alerts to the alarming situation regarding the subject and the importance of offering learning alternatives.

Various approaches have been proposed to overcome the learning difficulties, especially in the field of Chemistry.

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These strategies range from using scientific articles as teaching resources to carrying out practical experiments with everyday materials, to using different technologies to improve visuals and get students' attention [2].

The Brazilian Ministry of Education launched the Education Technology Guide in 2008 which describes a series of options for teachers to use in the classroom to enrich the pedagogical process. The use of technology is of great importance to the teaching and learning process, and this is happening rapidly. In 2019, the percentage of people who used the internet was 88.1% among students and 75.8% among non-students. In addition, the study found that among the population aged 10 and over, the main means of access was the cell phone (98.6%), followed by the microcomputer (46.2%), television (31.9%) and tablet (10.9%) [6].

Efforts are also being made to develop new pedagogical approaches that improve students' understanding since a large part of the topics studied in chemistry surround the understanding of chemical elements and their interactions. Although most of the elements are essentially three-dimensional, they are often presented in two-dimensional form through graphs and projections, which are difficult to understand and do not pose as a solution to the comprehension problem faced by students today [3]. The identification of chemical compounds is fundamental in the field of chemistry. However, the process of identifying these compounds can be a difficult task, especially when handwritten.

Considering this scenario, mobile applications serve to integrate technology into the students' learning process, given that they can be accessed by most students with devices within their reach. This could mean a positive scenario when considering the difficulties with students within chemistry, given that not only does mobile integration promote students' learning but it also affects their motivation [8].

III. MACHINE LEARNING

Machine learning is a constantly evolving sector among computational algorithms designed to emulate human intelligence by learning from the surrounding environment. They are considered the workhorse of the new era of so-called big data. Machine learning-based techniques have been applied in diverse fields, from pattern recognition, computer vision, spacecraft engineering, finance, and computational biology to biomedical and medical applications [4].

The intersection of machine learning and molecular chemistry education offers significant potential to improve teaching effectiveness by making learning more engaging, accessible, and tailored to individual needs. This innovative approach promises to transform the way concepts of molecular chemistry are understood in educational settings [5]. An example of the current use of machine learning in an educational setting is the identification of two-dimensional structure of mathematical symbols and expressions [15].

Among the variety of machine learning models, Supervised learning, the task function that maps an input to an output based on example input-output pairs, is widely used in detection models. It infers a function from labeled training data consisting of training examples. The basic flow of dynamics that occurs in supervised machine learning algorithms can be seen in Figure 1.

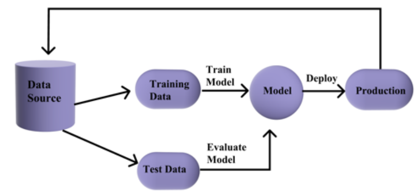


Figure 1. Dynamics In Supervised Machine Learning Algorithm.

This algorithm's main idea is to map inputs to the desired outputs modeling it through a function. This is regularly used in classification problems, so that the model must learn from a massive data source and, after being trained, outputs a classification for each of the inputs that are given to it.

Supervised algorithms are also defined by their classes, so any data that it collects will be classified into one of them [9]. These algorithms can also be combined with convolutional neural networks, in which there are different layers: an input layer, in which image data can be received, and the convolutional layer, which applies filters to the input and maps the produced outputs. Then there is a pooling layer, that performs a reduction to the spatial dimensions of the convolutional layer, reducing the number of parameters the model works with. Finally, the fully connected layers classify all the data passed to them and produce a final output [10]. A diagram of this process can be seen in Figure 2.

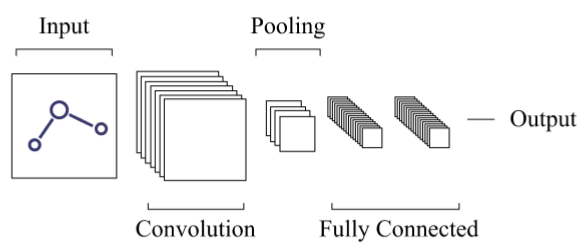


Figure 2. Diagram of a simple five-layered CNN architecture.

Supervised learning, combined with a convolutional neural network was an ideal structure for the machine learning model, considering the team's goal, which was to classify photos of a set of hand-drawn chemical molecules, as there is a standard for drawing them, so the model could use predefined data to predict new image occurrences.

IV. DEVELOPMENT

The development of the application, with its machine learning model, was accomplished using Apple Inc.'s Core ML framework [12]. This framework works together with Create ML, a platform designed for training models that seamlessly integrates into iOS and iPadOS applications. The image classifier within Create ML is designed to match images with predefined labels, efficiently determining the most suitable one for each image, by applying some of the machine learning techniques discussed previously.

The team adopted the Challenge Based Learning (CBL) methodology for this project, fostering collaborative efforts across its three main phases: Engage, Investigate, and Act. This structured progression provided a systematic approach to the research, enabling effective problem-solving [11].

The first phase (Engage) involved gathering ideas related to the central topic of research, involving the identification of problems that pose challenges. After determining the topic, the group proceeded to choose specific problems and proposed challenges aimed at alleviating or resolving them. The main research question emerged: "How to improve the learning of Chemistry through the use of Machine Learning?".

This central challenge guided the team into the Investigate phase. Now, the focus was on exploring resources to define the problem and propose solutions. Additional guiding questions also emerged, such as: "What are the best methods to optimize student learning?", "Does interactive learning enhance subject comprehension?", and "How can machine learning be effectively used to improve education and be made accessible to students globally?" The concept of an app that uses a camera to identify chemistry molecules stemmed from this phase, with each aspect of the app's development rooted in these formulated questions and emerging answers.

The final phase of the CBL, Act, involved the start of the training of a test model using Create ML. This phase aimed to test the feasibility of the gathered ideas for a solution. It was decided that all photos used to train the model would be taken from regular smartphones and later shared between the team. They consisted of hand-drawn molecules on plain white paper, whiteboards, and ruled paper.

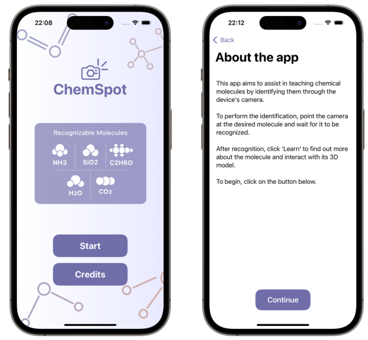
A Core ML model with images of water and silicon dioxide was generated, allowing the team to import it into any project supporting the Core ML framework. This initial model had the intent of evaluating how well the app would distinguish molecules that had similar structures. Our pilot tests exhibited reasonably high accuracy (82%), considering it was trained with just a small set of images. As the dataset expanded, the model's accuracy improved significantly, prompting further training to identify additional molecules.

After acquiring over two thousand images and importing them into Create ML, the final Core ML model was achieved. This model was integrated into an iOS app: ChemSpot, designed and developed to provide comprehensive information about the trained molecules. This app empowers students to identify drawn molecules and explore their properties, formulas, facts, and real-world occurrences.

V. RESULTS

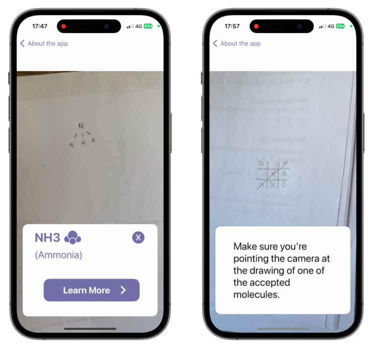
The entire process of training the model, designing, and developing the application was done in a single weekend, with further minor improvements. The CBL methodology was closely followed by the team and the app is currently still in development.

The molecules that the model was trained to recognize are shown right when the application is opened. They are H_2O (water), CO_2 (carbon dioxide), NH_3 (ammonia), SiO_2 (silicon dioxide), and C_2H_6O (ethanol). Those were the chosen molecules for the development of the app given their wide use and occurrence during the teaching of chemistry. Besides those molecules, two additional labels were implemented, so that the model could recognize drawings that were not one of the trained molecules so that the app would not display results.



(a) (b)

Figure 3. (a) Onboarding Screen with List of Recognizable Molecules and (b) Instructions Screen.



(a) (b)

Figure 4. (a) Process of scanning a hand-drawn molecule and (b) state when no molecules are recognized.

(a) (b)

Figure 5. (a) and (b) Learn More page presents the user with relevant information about the scanned molecule.

After clicking "Start" (*Figure 3a*), there is an introduction about the app and its main purpose: recognize hand-drawn molecules and provide useful information about them. This next screen (*Figure 3b*) also offers tips on how to get a better chance of the app recognizing a molecule. The user is then directed to a scanner, using the phone's camera, to identify any of the available molecules and is prompted to learn more about them (Figure 4).

When the user scans a drawing that appears not to be one of the molecules that are recognizable by the app, they are alerted of that, suggesting that they may be pointing to something that the app cannot recognize. When a molecule is recognized and the user clicks on “Learn More”, they are presented with detailed information about the molecule, accompanied by an interactive 3D model of it (Figure 5).

This demo app was created for iOS devices, for testing purposes and so that the app could be run on a phone (Figures 3 to 5), for practicality, or a tablet (Figure 6), where information can be better distributed, due to the larger display.

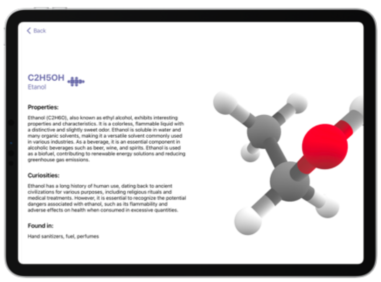


Figure 6. iPad app version of the Learn More page, showcasing a larger interactive 3D model.

Allowing users, especially students, to easily identify hand-drawn molecules and access relevant information about them can be a catalyst for making the study of Chemistry much more interactive and engaging for students. Apps can follow this approach to offer even more resources for students worldwide and create new experiences that aim to improve education.

Although the paper outlines a novel approach and the application seems promising in pilot tests, the full impact and efficacy of the tool will be more accurately gauged with comprehensive user engagement data and a broader dataset for model training.

VI. Conclusion

Technology was a great way to enhance the teaching and learning processes, by providing new ways for students and mentors to search for and interact with new topics and subjects. The pedagogical possibilities it offered were endless, and one of them was bringing interactivity into studying. In the Brazilian scenario, where laboratories were scarce in public schools and the average score for Chemistry in ENEM was below 50%, there was plenty of room for new ideas that aimed to improve the educational system.

This paper showed how machine learning, combined with mobile applications, had the potential to create powerful tools to assist the process of learning, through a demo app that identified hand-drawn molecules and provided information about them, including their properties, curiosities, where they could be found and an interactive 3D model, offering visual aids for the user, which had shown to improve the understanding of abstract subjects greatly.

The app’s model was trained to identify five molecules, but by training it further, more molecules could be implemented. Improvements to the information presented after scanning a molecule, like referencing other learning resources were also a future goal.

Lessons learned from initial failures, such as the challenges of accurately classifying molecules from hand-drawn images and the type of background they were drawn to, reinforced the need for a robust training dataset, which can be seen as future work. The project also highlighted the importance of user interface design that accommodates a wide range of users, from beginner to advanced students.

The use of machine learning for interactive educational tools in chemistry represented a new frontier in pedagogy, especially as it pertained to visual and interactive learning in the Brazilian context.

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