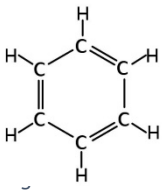

Molecules and Machine Learning:
Image Classification for an AR-Enabled Chemistry Classroom.

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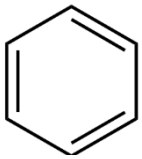

Figure 2 Benzene

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Abstract:

In coordination with augmented reality (AR), object recognition using artificial intelligence (AI) and machine learning (ML) have the potential of creating a new way of interacting with the world, particularly in the field of education. A mobile device's camera can view a scene, and AI algorithms can identify objects such as trees or chairs within the scene without user interaction. Using an automated machine learning (AutoML) tool, our research team will train a model and utilize that model in a real time, in conjunction with an AR application that will help chemistry students understand molecular structures. The input to the application will be an image, hand-drawn or computer generated. The app will run the image through our trained model, label it, and use that label to generate an interactive 3D model of the molecule. Initially, our research will train models for small datasets and evaluate the recognition results.

Introduction:

Learning chemistry requires the integration of information from macroscopic, microscopic, and symbolic domains of the discipline (1). The learning process is further complicated by abstract nature of chemistry concepts. The use of molecular models makes concepts more concrete by providing a representation of the microscopic domain (1). Our work will transform 2D compounds into interactive 3D, AR representations.

With the help of AutoML, our ambition is to build an AR tool for students to utilize alongside a lecture, almost like a private tutor in the student's pocket. When using AI, it is best to supply viable training data that closely matches the data on which predictions are to be made (2). Therefore, our initial repository will consist of a small number of both hand-drawn and computer-generated images of very distinct molecules. The immediate goal is to create a trained model that will recognize an image previously unknown to the model based on its distinguishing features. When the app recognizes the structure, we will link the object to a database that holds information about the molecule, and display an interactive 3D image in AR.

Machine Learning:

Traditionally, computer software algorithms use looping and branching to model repetitive and predictable processes where decisions are made on unambiguous data. Not all processes follow immutable rules, and not all decisions in the real world lead to a single unequivocal answer. Decisions made in ML systems are made on incomplete information. When using ML for image classification, the results are assigned a probabilistic value indicating the potential content of the image (3).

Machine Learning in Education and Chemistry:

ML currently has a positive impact in the educational field, for example, in the project Eduband, class content is adapted to each student – individually – based on their reactions (3). Another example is the platform Duolingo, which is used to learn new languages by studying

the learning behavior of each student and adapting the learning material to the needs of that individual (4).

There are numerous ways that AI applications are used in chemistry. One application uses ML to construct quantitative structure-activity relationship models (QSAR). QSAR models help to find relationships between chemical structures and biological activities of studied compounds (5). A second application utilizes a deep-learning method to identify the molecular structure of natural products. A program called SMART (Small Molecule Accurate Recognition Technology) was able to accelerate the identification process of a molecular structure by using recognition software to identify key pieces of information to obtain the structure of the molecule (6).

AutoML:

The purpose of an AutoML tool is to enable developers with limited machine learning expertise access to train high-quality models specific to their needs (7)**.** The goal of AutoML is to produce a machine learning model of a physical object or a label, using many images of the object or concept as input. A trained model has the capability to determine similarities in structures and can separate the parameters of the object from the surrounding scene. For example, a real estate company needs to split houses by category of ranch style home, apartment, and two-story home. An AutoML tool allows that company to upload images, train and validate a model, and release the model for use in applications. The process is outlined in Figure 3 below.

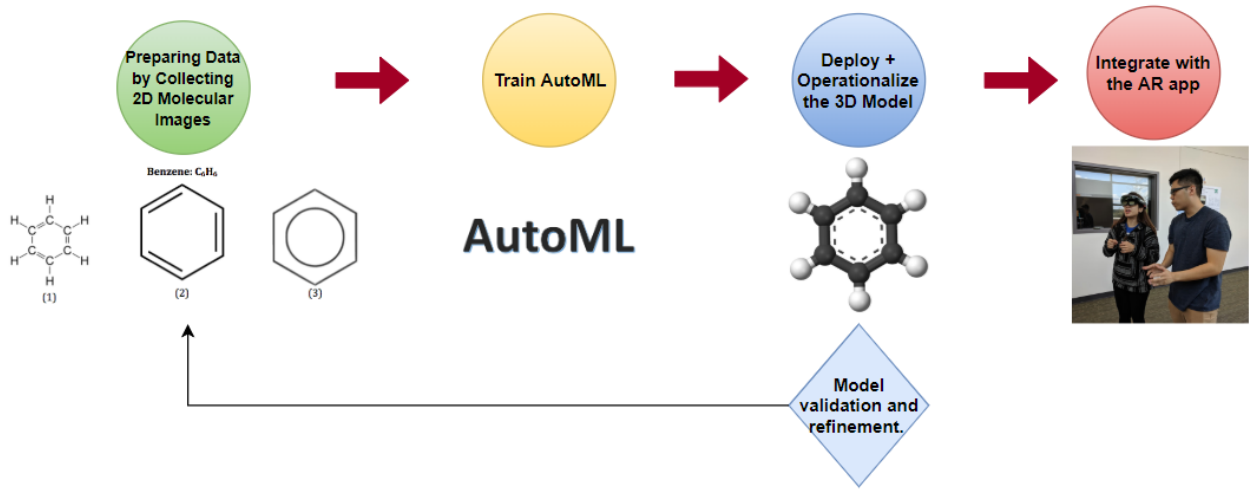

Figure 3: Process flow for training an AutoML tool.

Project Plan:

Initially our work focuses on preparing the model using AutoML. First, a repository of hand-drawn and computer-generated images are collected for a pair of very different molecules. The training process takes place and involves uploading the variety of representations (in an image format) of the molecular structures to the model. Then AutoML autonomously validates and tests the accuracy of the image recognition process. Ideally, afterwards, the model will recognize previously unknown structures and label the images appropriately. We will present our findings on the accuracy of the process flow depicted in Figure 3.

Future work involves increasing the number of molecules that the model can recognize, and integrating the AutoML image classification functionality as the input to present a 3D, AR rendition of the molecule. Finally, we want to help ensure the continued growth of the AutoML community by donating our data set to the open source Kaggle library.

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