



A Mobile App for Exploring Chemical Molecules:

Machine Learning-Powered Handwritten Compound Identification and 3D Visualization

Authors:

Luiza Coelho de Souza
Pedro Henrique Peraçoli Pereira Ceccon
Raphael Ferezin Kitahara
Silvana Rodrigues Alves

Presenter:

Name: Raphael Ferezin Kitahara
Affiliation: Eldorado Institute of Research, Campinas, Brazil
Email: raphael_kitahara@hotmail.com



Resume:

I am Raphael Kitahara, 20 years old and a student of Computer Engineering at the State University of Campinas (UNICAMP).

Among my interests are app development and design.



Enhancing Chemistry Education with Technology

- **Challenge:** Chemistry, a core subject in Brazilian basic education, is often seen as difficult and abstract by students. This perception leads to resistance in learning and understanding its real-life applications.
- **Limitations of Traditional Learning:** Laboratory practices, though effective, are not always feasible due to the lack of facilities in many schools and the constraints of online learning.
- **Innovative Solution:** Development of a mobile application using machine learning.
- **Key Features:**
 - Identifies hand-drawn molecules through user input.
 - Generates 3D virtual models of molecules, providing a dynamic visual learning tool.
 - Offers detailed information linking chemical elements to everyday life applications.
- **Impact:** This approach aims to make chemistry more accessible and engaging, transforming abstract concepts into tangible and relatable knowledge.



Challenge in Chemistry Education

- **Difficulty in Learning:** Chemistry is often perceived as an abstract and challenging subject by students.
- **Lack of Resources:** Many schools lack the necessary infrastructure to conduct laboratory experiments, especially during online classes.
- **Need for Innovation:** There is a critical need for innovative solutions to make chemistry more engaging and accessible.



Bridging the Gap with Technology

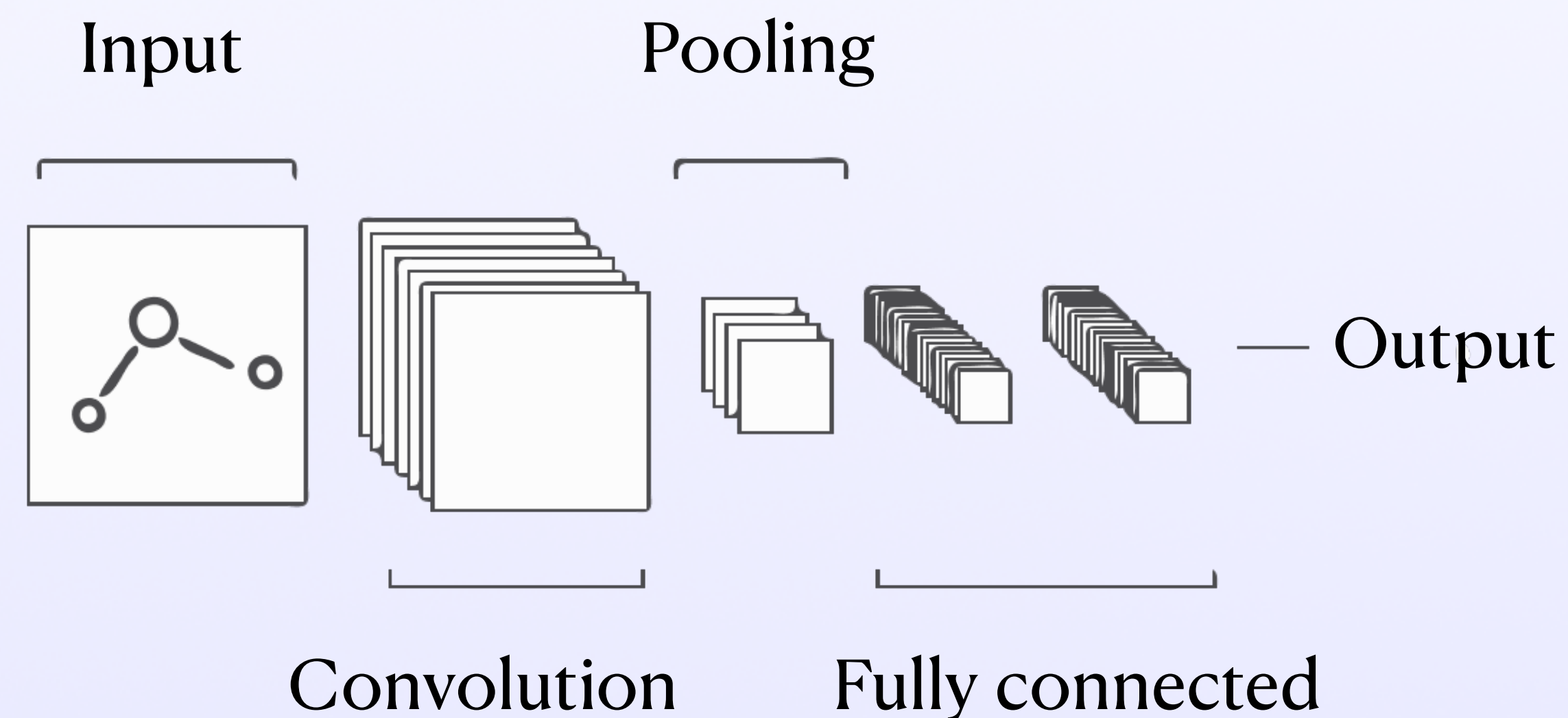
- **Mobile Learning:** Introduction of a mobile app as a solution to accessibility and engagement challenges in chemistry education.
- **Machine Learning:** Utilization of machine learning to identify hand-drawn molecules and present them as 3D virtual models.
- **Real-World Connection:** Providing contextual information that relates chemistry concepts to everyday life.

Machine Learning Model

The project employs Convolutional Neural Networks (CNNs), chosen for their superior performance in image recognition tasks, utilizing Apple's Core ML and Create ML for efficient model integration and training.

- **Training Process:** The training process began with an initial accuracy of 82%, which significantly improved as the model was exposed to a larger dataset.

This model has been seamlessly integrated into the ChemSpot app, enabling it to accurately identify hand-drawn chemical molecules, thereby enhancing the educational experience by connecting abstract chemical concepts with interactive and tangible visualizations.



ChemSpot: A New Way to Learn Chemistry

- **Development:** Use of Apple's CoreML framework for efficient machine learning model integration.
- **Features:** Ability to recognize various molecules and present them with informative content and interactive 3D models.
- **User Interface:** Designed for ease of use, encouraging self-led exploration and learning.

