DEEP LEARNING METHODS FOR THE IMAGE-BASED ASSESSMENT OF PHYSICAL STABILITY OF LIQUID FORMULATIONS

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A key aspect in the design of formulated liquids is ensuring physical stability over full shelf life. The process of physical stability testing of liquid formulations is a time-consuming task which is ubiquitous in all industrial sectors. Assessment of physical stability is typically done by placing finished products in transparent jars and observing those at given intervals of time. An observation is labelled as "pass" or "fail" or sometimes through loss of stability descriptors. Observations are typically run in real time by expert researchers and are recorded digitally. However, once done, the observation cannot be repeated anymore. In order to reduce the effort of stability assessment and automate the process, P&G is replacing the visual observation with a recorded image of sample, which could be graded at a later stage, guaranteeing the repeatability of the observation. To further automate and digitize the process, it is desirable to create a machine learning classification model.

Machine learning and deep learning algorithms have been widely used in many scientific areas, including chemical engineering sectors, as for modeling, optimization and control. Many industries have already implemented machine learning methods for economic optimization problems and research purposes. A tremendous amount of data is needed to achieve satisfying results.
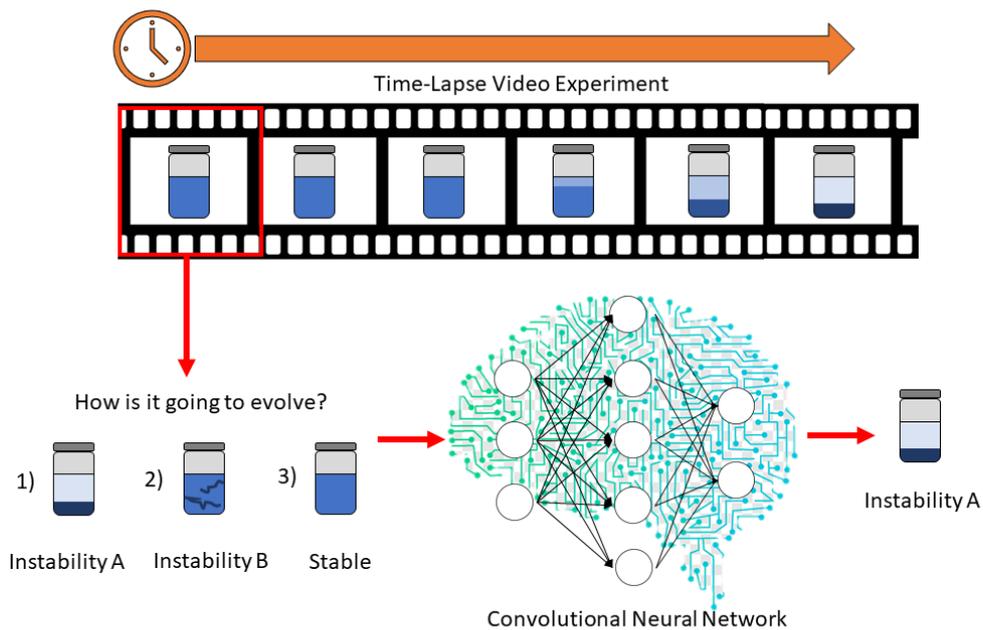
Among the learning techniques, supervised learning addresses the task of predicting labels given input features. This is done by feeding the algorithm a dataset of labelled examples. If the target is a continuous function, the algorithm is solving a regression problem; if the target is discrete, it is solving a classification problem. Convolutional Neural Networks (CNNs) are machine learning algorithms that apply convolutions in their layers to extract the most relevant features.

The goal of this PhD thesis is to propose novel and effective methods for the analysis of fluid stability, based on time-lapse photography and Artificial Intelligence. Starting from a large amount of data labelled by expert analysts, suitable deep-learning architectures will be developed and trained to classify the current state of fluid vials and predict their future evolution.

The first year of the PhD has been entirely devoted to the study of machine learning theory and methods, as well as the implementation in Python programming language of some basic convolutional neural network architectures. A background of programming skills in Visual Studio was also required to code windows apps. To speed up the labelling process an app was developed.

The second year is focused on the generation of a labelled dataset and on the implementation of deep learning algorithms, mainly CNNs, in order to develop a model capable of classify the instabilities of formulated liquids with a sufficient level of robustness.

The third year will be focused on the prediction of the evolution of those formulated liquids.

Dottorato in Ingegneria dei Prodotti e dei Processi Industriali

Time-Lapse Video Experiment

How is it going to evolve?

1) Instability A 2) Instability B 3) Stable

Convolutional Neural Network

Instability A

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