Cancer Biomarker Detection and Classification: Extracellular Vesicles, Raman Microscope and Convolutional Neural Network

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Abstract

Raman spectroscopy probes molecular vibration and thus reveals chemical information of a sample without labeling. This optical technique can be used to study the chemical composition of Extracellular vesicles (EVs). EVs are tiny spherical particle realized by all kind of mammalian cells. The particles are involved in inter cellular signaling, garbage management, cancer metastasis and so on. EVs have a complex chemical structure and heterogeneous nature. Therefore, we need a smart way to analyze/classify the EVs' Raman spectra. Machine learning (ML) can be a solution for this problem. In this research, we applied convolutional neural network (CNN), which is one of the ML algorithm, to classify the EVs' Raman spectra.

With Raman optical tweezers, we obtained Raman spectra from four EV subtypes -red blood cell, platelet, PC3 and LNCaP- derived EVs. To classify them by their origin, we used CNN. We adapted the CNN to one dimensional spectral data for this application. The ML algorithm is a data hungry model. The model requires a lot of training data for accurate prediction and avoiding overfitting issue. To further increase our substantial dataset, we performed data augmentation by adding randomly generated Gaussian white noise. The model has three convolutional layers and fully connected layers with four hidden layers. The Leaky rectified linear unit and the hyperbolic tangent are used as activation functions for the convolutional layer and fully connected layer, respectively.

In previous research, we classified EV Raman spectra using principal component analysis (PCA). PCA was not able to classify raw Raman data, but it can classify preprocessed data. CNN can classify both raw and preprocessed data with an accuracy of 93% or higher. It allows to skip the data preprocessing and avoids artifacts and (unintentional) data biasing by data processing.

Keywords: *Extracellular Vesicles, Raman spectroscopy, Machine learning, Convolutional Neural Network, Cancer, Biomarker*

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Biography

Wooje Lee graduated from Myongji University, South Korea, receiving a BSc in Electronics Engineering. In August 2015, he received MSc degree with a topic of Ion Sensitive Field Effect Transistor Based pH Sensor Development for Internet of Things in Electronics Engineering under the guidance of Professor Sang Jeen Hong at Myongji University. In September 2015, he started his PhD degree in Optical Sciences group at University of Twente, Enschede, the Netherlands. During his doctoral trajectory, he