Chapter 3
Machine Learning Applications in Nanomedicine and Nanotoxicology: An Overview

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ABSTRACT

The development of machine learning algorithms together with the availability of computational tools nowadays have given an increase in the application of artificial intelligence methodologies in different fields. However, the use of these machine learning approaches in nanomedicine remains still under-explored in certain areas, despite the development in hardware and software tools. In this review, the recent advances in the conjunction of machine learning with nanomedicine are shown. Examples dealing with biomedical properties of nanoparticles, characterization of nanomaterials, text mining, and image analysis are also presented. Finally, some future perspectives in the integration of nanomedicine with cloud computing, deep learning and other techniques are discussed.

INTRODUCTION

Nanomaterials have arisen as one of the promising fields in material sciences and technologies in the current century. The most prominent that should be mentioned include among others the development of new fuel cells (Liu, Ling, Su, & Lee, 2004), electronic devices (Novoselov et al., 2012), coatings (Ragesh, Anand Ganesh, Nair, & Nair, 2014), diagnostic imaging (Wu et al., 2002), and drug delivery (Muller & Keck, 2004). The field of nanomedicine has gained a great importance in the last years. In the case of nanomedicine successful applications of computational approaches, most of them related with QSAR (quantitative-structure activity relationships) studies.

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In this sense in this review we cover the main applications of machine learning methods in medicine, where the most relevant publications are discussed for this field. This has led to the development of different approaches, based in the predictions of the effects of nanoparticles, the enzyme inhibition of carbon nanotubes and others in the use of artificial intelligence for the study of nanoimages to predict the response to certain effects, or the improvement of personalized cancer treatment based in nanometer-scale drug delivery systems.

The State of the Art of Machine Learning and Nanomedicine

In the era of data, machine learning (ML) algorithms have played a crucial role by helping to improve the predictions of biological, physical, chemical and toxicological effects. As the size of the information increase these artificial intelligence methods are of valuable important to analyze this huge amount of data.

One of the main practical use is for virtual throughput screening of new chemical entities, based on the information gathered from previous one. A common procedure to perform this kind of study is by the Quantitative Structure-Activity Relationships (QSAR) methods, a statistical method, in a general way which try to correlate the biological effect with the features describing the compounds, molecular descriptors gathered directly from the chemical structure through mathematical equations of the connectivity graph. In the case of nanomaterials other descriptors can also be obtained like shape, size, composition, surface modifications, and propensity to agglomerate, interaction with different molecules, and aqueous solubility that could influence the properties of the nanomaterials affecting the biological responses.

The impact of this field was analyzed by retrieving in the Scopus database a search using the search criteria “Machine Learning” AND “Nanomedicine”. As can be observed in Figure 1 the time period for Machine Learning-Nanomedicine search comprises the time period from 1999-present, with 921 documents this is compressible because this is novel multidisciplinary field. As can be noted a constant increased in this field is observed. From this could be said that this thematic constitutes a hot topic nowadays due to the increased interest in drug discovery and design.

Figure 1. Yearly publications based on ‘Machine Learning’-‘Nanomedicine’ keywords