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Editorial

Chemoinformatics and Artificial Intelligence in Biochemistry

Ramzi El Feghali[1,2]* and John Kahura[1]

[1]*AIIHC International Ltd., London, United Kingdom*

[2]*Main Office: Building Elias Feghali, Bsous, Lebanon*

***Corresponding author:** Ramzi El Feghali, AIIHC International Ltd., 27 Old Gloucester Street, WC1N 3AX, London, United Kingdom and Main Office: Building Elias Feghali, Bsous, Lebanon.

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Editorial

Chemoinformatics is an emerging field since the end of 1990s, which has involved different methods from the artificial intelligence technology mainly around the years 2010s, when the deep learning application in chemistry and biochemistry allowed to the chemists and biochemists to draw precisely for the first time, the chemical structure of different atoms, and molecules in structural chemistry and biochemistry, and to reproduce many chemical reactions in general and organic chemistry but mainly in biochemistry for fundamental, pharmaceutical and medical purposes.

During the past years, descriptive and inferential statistics, have been reinforced by large-scale data analysis and meta-analysis methodologies presenting a better understanding of the data in the frame of a data mining process to understand the chemical mechanisms generating this data, where the progress in computer science frameworks and algorithms has contributed deeply to organizing those different chemical systems as well as their digitization (e.g. glucose metabolism in a cell, oxidation-reduction reactions, atoms and molecules structures). The big issue encountered during those first years, was generating complete unbiased data by the intermediate of chemical in vitro experiments, allowing the different algorithms and models to generate unbiased forecasts and inferences based on the experimental data (e.g. secondary and tertiary structure of a protein, efficiency of a molecule in healing a disease, interaction between different molecules in the blood).

While the field of chemistry and biochemistry was evolving to fix this issue related to the missing values or the bad quality of collected data from controversial chemical reactions and experiments, artificial intelligence [1,2] was introduced to the chemistry field, by the intermediate of the supervised machine learning and deep learning neural networks algorithms, allowing to standardize and digitize in silico many of those chemical reactions (e.g. protein-protein interaction, drug/protein molecule docking, chemical reactions' catalyzer identification in silico) allowing even to those algorithms to simulate virtually new chemical reactions by the intermediate of generative neural networks, based on existing ones used to train "teach" different statistical and algorithmic models used in artificial intelligence, to be able then to predict the outcomes in different fields of chemistry (e.g. chemical kinetics, electrochemistry, equilibrated reactions).

In summary, supervised machine learning [3] and deep learning [4,5] are algorithmic methods based on a training set of data and an experimental set of data, allowing them to develop a model following different steps. The first step is to train the supervised machine and deep learning algorithmic models based on mathematical methods of linear and nonlinear regression, hyperplanes, metrics, thresholds, multi-layers, and calculation loops allowing those algorithms to calculate mathematical scores from those training databases and to create the nodes of the neural networks [6] successively used as a reference to classify in a second step the data of the experimental set into groups called classes or classifiers. As an example, based on a training database in medical biochemistry, there won't be just one threshold as we can see today in the laboratory medical and biological analyses report (a value, or a range of values) to identify a metabolic disease (e.g. 1mg/dL for the glucose's level in the blood) but different thresholds related to the subgroups of patients used to train the machine/deep learning algorithms (e.g.: 0.8mg/dL "blood glucose level" in diabetes, and 0.9mg/dL "blood glucose level" in obese patients).

We won't extend the application of artificial intelligence to medical imaging, in this editorial, where it has been well developed since the end of the 1990s mainly for the diagnosis of cancers (brain, lung, breast, pancreatic, stomach, and other type of cancers), we'll just mention the fact, that today deep learning is used for preventive diagnosis in medical imaging based on micro-discrepancies identified by the algorithms in the radiography or tomography images, the first stages of a cancer, much easier to treat than the late stages of a metastasis. Also some deep learning developments based on the recursive neural networks (backward technique), allow the algorithms to not just answer to different questions the way the convolutional neural networks (forward technique) do based on a training set, but from a single picture (e.g. metastasis radiography or tomography) a pretrained deep learning model from a training set of information (colors, positions, dimensions) can redraw, by generating new sets of data, different cases of primary, secondary and tertiary stages leading to the metastasis. Those techniques can be as well used to redraw trees of words from a single phrase, or less precisely aleatory threshold values from a single number.

For this reason, we could see, that since the years 2000s, machine learning (support vector machine, self-organizing maps, decision trees, naive Bayes) followed by the deep learning [7,8] have been massively deployed in the different branches of chemistry and biochemistry to reproduce and simulate in silico different chemical experiments and to classify different animal models and human diseases based on those reactions into groups (e.g. comparison of the metabolic systems in mouse model vs human being, personalized diagnosis of a disease in a human model). The coding languages mostly used today to implement those algorithmic models in artificial intelligence (machine and deep learning) and currently using them, are mainly the statistical R language and Python language where many packages, libraries and frameworks have been developed since the end of the 1990s (Tensorflow, PyTorch, Keras, Django, Flask).

AIIHC International Ltd. Is a Lebanese-British company having its offline team based in Lebanon and its headquarters in London, Grand Britain. Besides, the services we are offering in statistics, and big data analysis, we are developing a platform on our domain *https://aiihc.com* publishing E-Learning courses (files and videos) in Artificial Intelligence applied to HealthCare as well as consultancies in the field of chemistry, biochemistry, statistics and artificial intelligence, via a videoconferencing and a forum spaces. Finally, a brand OmiXDiaG® is under development implementing the machine and deep learning in different fields of chemistry and biochemistry applied to healthcare, mainly in phytotherapy (OmiXDiaG® Phyto.), music therapy (OmiXDiaG® M.T.) and pharmaceuticals (OmiXDiaG® Pharma.). Weekly podcasts, webinars, workshops and conferences are taking place since 2022, most of them are free presenting to the students and professionals of healthcare the technologies of artificial intelligence, coding sessions under R and Python, as well as the application of machine and deep learning algorithms in the different fields of basic sciences and healthcare. The difference between our platform and other social media or educational platforms is that many apprentices can join it without paying any fees and focus on the field of artificial intelligence without distraction with other general news and without paying any expensive fees like it's the way with other programs less complete than our platform. More, as experts in the field of machine learning and data analysis applied to healthcare, we are a team of data scientists with chemistry and biochemistry background, software engineering and business development, in case the apprentices and healthcare professionals, would like to launch a career as entrepreneurs they can benefit from a free coaching and consultancies in artificial intelli-gence and business development. The platform for regulation matters is accessible today all over the world except in 3 regions: Europe, North America and Australia, but we are programming to extend to those regions in the future.

Finally, as this field of digitization and chemoinformatics is at its beginning, the horizons of this field remain unknown and invisible yet. So, maybe all together as AIIHC Team, our leads & partners will be able to reach those boundaries in the coming years offering to the healthcare community and professionals, new solutions to improve the sector of health. Finally, with AIIHC you can better see, AIIHC will take you beyond the sea, "Our Slogan".

Acknowledgments

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Conflict of Interest

None.

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