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Editorial

BioMedInformatics, the Link between Biomedical Informatics, Biology and Computational Medicine

Alexandre G. de Brevern ^{1,2}

¹ Université Paris Cité, INSERM, BIGR, DSIMB Bioinformatics Team, F-75014 Paris, France; alexandre.debrevern@univ-paris-diderot.fr; Tel.: +33-1-44493000

² Université de la Réunion, INSERM, BIGR, DSIMB Bioinformatics Team, F-97715 Saint-Denis, France

1. Why a Journal Named “BioMedInformatics”?

Welcome to *BioMedInformatics* (ISSN: 2673-7426). As its title suggests, this journal bridges the gap between medical science and new developments in bioinformatics in all its forms. This young journal, created in 2021, was fortunate to have had an excellent start under the editorship of Professor Jörn Lötsch (Goethe-Universität Frankfurt am Main, Germany) [1]. I had the honour of succeeding him in March 2023. In this short time, *BioMedInformatics* has already published over 130 articles and reviews, and has been recently indexed by SCOPUS.

Let me highlight the key points of the journal’s scope and philosophy to demonstrate why *BioMedInformatics* is the ideal place for your work on all areas of biomedical informatics, as well as computational biology and medicine. Medicine is the science of maintaining and restoring health, while bioinformatics can be defined as the application of computational and analytical tools to the acquisition and interpretation of biological data. It is an interdisciplinary field that utilizes computer science, mathematics, physics, chemistry and biology. Following the completion of first human genome, more than 20 years ago, Ardeshir Bayat shared his thoughts [2] on the link between medicine and bioinformatics: “As a result of this [completion], a whole new age of individually tailored medicine will emerge. Bioinformatics will guide and help molecular biologists and clinical researchers to capitalise on the advantages brought by computational biology”. Of course, it did not happen quite so quickly.

Figure 1 summarises the evolution of medical studies with the arrival of these bioinformatics and computational biology approaches. Traditionally, a doctor sees a patient with pathology and provides a treatment to cure the disease.

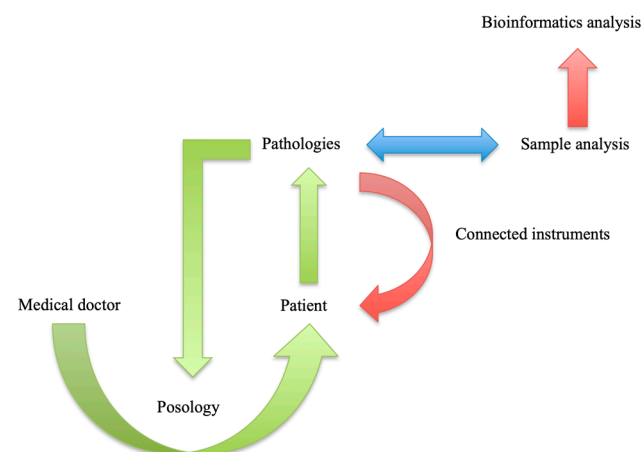


Figure 1. A brief summary of current medical analysis.



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To determine certain factors, additional tests may be carried out (e.g., urine or blood tests). Classical biochemical studies are used to determine the patient's pathology. Bioinformatics approaches have enabled new analyses to be carried out, as well as improving the follow-up of the patient's medical equipment. These analyses make it possible to locate new pathological players as well as to design responses more efficiently (e.g., drug design).

In the following section, we list some examples of papers that follow this typical *BioMedInformatics* research approach, especially concerning recent developments.

2. Some Relevant Examples from *BioMedInformatics*

2.1. Classical Bioinformatics Questions

Bioinformatics has often been used to discover oncogenic markers [3]. Mehmood and colleagues are interested in DNA methylation associated with breast cancer [4]. Mutations or aberrant expression of genes encoding regulators of DNA methylation can lead to the aberrant expression of critical molecules. Using genomic and transcriptomics data from The Cancer Genome Atlas (TCGA), Genotype-Tissue Expression (GTEx) and microarray platforms, the authors characterized several mutations in genes encoding the regulators of DNA methylation, showing significant differences between normal and diseased tissues. The deregulated expression of certain genes appears to correlate with patient prognosis. These results advance our understanding of the aetiology of the disease and could be used to identify alternative targets for new therapeutic strategies against cancer.

The term bioinformatics is often associated with finding a few genes involved in a metabolic pathway or cancer. It is less common to think of the possibility of finding information about psychiatric diseases [5]. Cao and colleagues present a fine-grained analysis of the genome-wide association (GWAS) study of dementia [6]. A key feature of the analysis was access to particularly well-monitored patients with electronic medical records that could be described as robust. The authors defined three decision rules for the discovery of significant SNPs for GWAS. They showed significant associations between TOMM40 protein variants and dementia. Some of these new potential SNPs for dementia are associated with brain or neurodevelopment, opening up possible avenues for further study.

In recent years, emerging infectious diseases (EIDs), whether of animal origin or due to the increased prevalence of existing human diseases, have posed significant challenges to public health and global security. The most obvious case is SARS-CoV-2. There is an urgent need for innovative and robust technologies to effectively monitor emerging pathogens. In the context of rapid identification, epidemiologic surveillance, as well as mitigation of transmission, genomics has become an essential public health tool in all phases of pandemics. Vashisht and co-workers have therefore written a review article that provides an overview of recent advances in various genomic techniques for detecting and monitoring pathogens and their applications in global epidemic surveillance [7]. In addition to a clear presentation of genomic analyses in understanding the epidemiology of emerging infectious diseases, they outlined the technical challenges and limitations, as well as ethical and legal considerations.

An essential axis of bioinformatics since its beginnings has been to support the annotation of biological data. An important example of this type of research is the IMGT (<https://www.imgt.org>, accessed on 13 December 2023) [8], a reference database on immunoglobulins for more than a quarter of a century, created by Lefranc and Lefranc. This database provided not only access to the data but also precise annotation with new rules. In their article for our journal, Lefranc and Lefranc focus on specific questions, identifying allotypes on the heavy chains gamma1, gamma2, gamma3 and alpha2 (known as G1m, G2m, G3m and A2m allotypes, respectively) and on the light chain kappa (Km allotypes) [9]. The Gm and Am allotypes are some of the most powerful tools in population genetics because they are inherited in fixed combinations or Gm–Am haplotypes (ref). They provide an important system for understanding the immunogenicity of polymorphic IG chains in terms of amino acids and conformational changes. The WHO/IMGT allotype nomenclature and the unique IMGT constant domain (C) numbering relate the Gm–Am and Km

alleles to the alleles and structures of the IGHC and IGKC genes and, by definition, to the immunogenicity of the IG chain, paving the way for immunoinformatics for personalized therapeutic antibodies and engineered variants.

2.2. Machine and Deep Learning Innovative Developments

The advent of new experimental methods has led to the generation of an increasing amount of digital information about the human genome and proteome, as well as a large number of resulting omics. In this context, artificial intelligence (AI), through machine learning (ML), artificial neural networks (ANN) and deep learning (DL), is now at the heart of biomedical research and has already paved the way for significant breakthroughs in biological and medical sciences [10]. AI and computation have transformed traditional medicine into modern biomedicine and promise a new era of systems biology that will improve drug discovery strategies and facilitate clinical practice. Athanasopoulou and co-workers therefore provide a concise review that allows a quick overview of the main categories of AI, with the basic principles of the widely used ML, ANN and DL approaches [11]. This review highlights the challenges and future directions of AI in modern biomedical studies.

While deep learning has taken an important place in classification and prediction, more general questions of basic research remain relevant. Thus, Lötsch and Ultsch focus on multinomial regression analysis to identify variables relevant to class structure in biomedical datasets [12]. Their work is part of this dynamic that tends not to use traditional regression analysis in biomedical research. Using artificial data and biomedical datasets from cancer research, they tested machine learning models such as random forest, support vector machine, Bayesian classifiers, k-neighbour closeness and repeated incremental cutting (RIPPER). These models consistently outperform regression by accurately classifying new cases. They draw parallels with the limitations of single-layer neural networks and conclude that regression per se is not the best model for class prediction in biomedical datasets. Particularly interestingly, they suggest that a “mixture of experts” approach may be a more advanced and efficient strategy for analysing biomedical datasets.

Myocardial infarction (MI) has a major impact on the global population. Myocardial infarction is the death of the heart muscle due to a lack of blood oxygenation and depends on a large number of factors and parameters [13]. An electrocardiogram (ECG) machine is undoubtedly the most effective way to monitor and try to prevent this type of pathology. Patients with MI need immediate intervention, as any delay will lead to worsening heart problems or heart failure. In this type of research, Hasbullah and colleagues developed a fast and reliable system to facilitate the automatic detection and prediction of MI from ECG readings [14]. Methodologically, they relied on a recurrent neural network (RNN) that learned data from various public databases after optimizing the ECG analysis parameters. They tested different types of architectures and showed, for example, that convolutional neural networks (CNN) also showed good results in solving prediction problems. Although CNN models do not have the ability to store temporal information, hybrid models of CNN and RNN techniques for MI prediction (e.g., CNN-LSTM and CNN-BILSTM) have been developed and show excellent results. The performance evaluation of different models shows an excellent overall accuracy of 89% for CNN-LSTM and 91% for CNN-BILSTM model.

Hong and Fenyö were interested in computational pathology [15], a discipline that involves the efforts of pathologists and computer scientists and has benefited particularly from advances in deep learning in recent years [16]. In this field, several models have also proven useful for clinical diagnosis based on histopathological images. Morphological features extracted from the model show correlations with molecular-level features, including unique mutations and subtypes, most of which were previously unknown to human pathologists and clinicians. Their review provides a good overview of this growing area of research. Of particular importance, Hong and Fenyö acknowledge the limitations and potential obstacles that prevent the implementation of these models in contemporary real-world clinical settings. For example, only models previously understood by pathologists

can be used as reliable predictive evidence, which significantly limits the tasks to which deep learning models can be applied. In addition, patient samples are also very limited for each of the specific tasks of interest. Labelling standards among clinicians also vary widely from country to country, further complicating the task.

Uterine endometrial carcinoma (UCEC) is unfortunately the second most common gynaecologic cancer worldwide. Anachronistically, the number of UCECs is increasing even though no significant progress has been made in the field recently. There is an urgent need to identify novel biomarkers for UCEC. In this context, Fu and his colleagues were interested in disulfidptosis, a novel form of cell death [17]. However, its role in UCEC is unclear. Fu et al. applied differential analysis and the XGBoost algorithm to patient data from The Cancer Genome Atlas (TCGA). Among the ten characteristic genes associated with disulfidptosis (DRG), they were able to select one of interest. The identification of LRPPRC as a DRG allowed them to construct a ceRNA regulatory network associated with LRPPRC, consistent with the scientific hypothesis. Then, they constructed a risk prediction model with good predictive performance based on seven disulfidptosis-related characteristic lncRNAs (DRCLs) and proposed 14 small molecules as potential drugs for UCEC treatment. Finally, they identify the typing of DRG and DRCL and explore their biological characteristics. The results have potential theoretical implications for improving the survival rate and treatment effect of UCEC, thus promising to contribute to research and clinical practice.

2.3. Classical Bioinformatics Questions

The (3D) structure of proteins is of great interest in both basic and applied research, but identifying it can be complex, time-consuming and expensive. Therefore, *in silico* computational approaches are an attractive and sometimes unique alternative. In this context, the AlphaFold2 protein structure prediction method [18] represents a revolutionary advance in structural bioinformatics. Named Method of the Year 2022 [19] and widely used by EBI (<https://alphafold.ebi.ac.uk>, accessed on 18 December 2023), it was thought that protein-folding problems had been solved. However, the reality is more complex. Due to the lack of experimental input data, combined with crystallographic challenges, some goals remained very difficult or even unattainable. Tourlet and colleagues present in this review a perspective dedicated to a non-expert audience, discussing and correctly placing the AlphaFold2 methodology in its context and, above all, highlighting its use, its limitations and its opportunities [20].

From a pharmaceutical point of view, transmembrane proteins (TMPs) represent an important class of proteins (more than half of the therapeutic targets), but the difficulty of obtaining structures remains a major problem. Also, the proposal of structural models remains a major axis of research. However, few approaches are specifically dedicated to them and in particular to the evaluation of the quality of TMP models [21]. Télétchéa and collaborators have therefore developed a specific method called HPMScore [22] (https://www.dsimb.inserm.fr/dsimb_tools/hpmscore, accessed on 17 December 2023). It takes into account sequence and local structural information using the unsupervised learning approach called the hybrid protein model. The method was extensively evaluated on very different TMP all- α proteins. The HPMScore achieved better results than DOPE, the most widely used approach, in identifying good comparative models compared to more degenerate models, with a top value of 46.9% versus DOPE 40.1%. A dedicated web server has been set up and made available to the scientific community. It can be used with structural models generated from comparative modelling to deep learning approaches such as AlphaFold2.

Like all fields, drug discovery is also affected by deep learning [23]. Therefore, Matsuzaka and Yashiro have made a short and instructive review to outline the knowledge on the applications of deep learning for drug discovery systems with big data [24]. After presenting the question of the architecture of these approaches, they show the problems related to this type of research and then provided sets of relevant research in the field,

also raising the crucial question of the relevance of the evaluation of these approaches in this domain.

Askari and colleagues make the same kind of argument, but specifically for biosimilars [25]. A biosimilar drug is simply a biological substance that is similar to the reference drug. It must have no clinically significant differences in potency, purity or safety compared to the original drug. This area is extremely active due to the financial implications of this type of research. The strategic use of computational methods accelerates the discovery and optimization of biosimilar candidates and provides insight into their safety, efficacy and structural similarity to reference molecules; these typically include molecular modelling and simulation, virtual screening and QSAR modelling. AI is gradually being integrated but has not yet led to advances as significant as AlphaFold2. The authors show that the future of biosimilar development will thus reshape the approach to biosimilars and the broader frontiers of pharmaceutical progress.

2.4. Dealing with the Patients

Clearly, thinking about a patient's quality of life does not often bring video games to mind [26]. However, Lima and colleagues propose a strict protocol for evaluating the effectiveness of using Wii games in the physical and functional training of the elderly [27]. In this age group, there is often a decline in exercise capacity and a reduction in muscle strength, flexibility and bone mass, leading to poor locomotion, lack of balance and falls. Exergames therefore represent an interesting possibility. They are the result of technological advances and offer users an interactive environment that combines play with physical and cognitive exercise, and Wii games are well represented. The details of the protocol show the complexity of the question raised.

Similarly, bedridden patients are at risk for several problems caused by prolonged immobility, resulting in a prolonged recovery process. Neves and colleagues propose a project called ABLEFIT to develop a medical device for the physical rehabilitation of bedridden patients with prolonged immobility [28]. To this end, they developed a prototype to monitor several parameters and statistically evaluated a user-centred multi-method approach (user-centred and human-centred design) to evaluate the functionality, ergonomics and safety of the device. This monitored and computerized study showed the importance of joint stabilizers, heart rate and SPO₂. An important concern for the ergonomics and performance of the caregivers was also implemented, providing a dynamic solution (using gamification and simulation technologies) and allowing the generation of personalized rehabilitation plans.

Saber Amsalam and colleagues solved a complex problem in Iraq by automatically detecting facial paralysis, age and gender using a Raspberry Pi [29]. They proposed a complete recognition and detection system with a small portable system. Facial paralysis is a neurological disorder that affects the facial nerve, causing the patient to lose control of the facial muscles on one side of the face. Diagnosis by visual examination, based on differences between the sides of the face, can be subject to errors and inaccuracies. A deep learning approach was also used to propose a system for the real-time detection of PF and determination of the patient's gender and age from a local data bank of more than 20,000 images. The Raspberry Pi was equipped with a digital camera and a deep learning algorithm. The method achieved a prediction accuracy of 98%. The solution facilitates the diagnostic process for both the doctor and the patient and could be used as part of a medical assessment activity.

This type of approach is also useful in the context of arrhythmia problems. The Holter electrocardiogram (ECG) is one of the most classic measures of cardiac monitoring, both in patients simply considered at risk and in those with cardiac hypertrophy. It has been shown that myocardial remodelling, which occurs with age or after myocardial infarction, can lead to drastic fluctuations in the length of the cardiac pulse interval. The presence of these abnormally high heart rate variations increases the risk of fatal arrhythmia events. The ECG provides a long signal that represents the heart's responses to both autonomic

regulation and various phenomena, including the remodelling of cardiac tissue. Makowiec and co-workers are doing important modelling work here, symbolizing the ECG through acceleration and/or deceleration patterns, which allows the use of entropic measures to evaluate the complexity of the heart rate [30]. They visualized the pattern dynamics of the entire signal and analysed the signal to find the pattern dynamics in a sliding window. The method was applied to a cohort of heart transplant recipients (HTX) divided into the following groups: a left ventricle of normal geometry (NG), concentrically remodelled (CR) and hypertrophically remodelled (H), and a control group (CG) composed of signals from 41 healthy contemporaries. The visualization of the dynamics of the group patterns showed severely limited autonomic regulation in HTX patients compared to CG. The analysis (in segments) proves that the configurational dynamics of the NG group is different from the configurational dynamics observed in the CR and H groups. Thus, the dynamic entropy estimators tested in moving windows detected the left ventricular remodelling in stable HTX patients.

Of course, these articles represent only a small number of the diverse manuscripts published by *BioMedInformatics*, but they are good representatives of the dynamics of the field, which combines both age-old medical questions and the latest discoveries in learning techniques.

We would also like to take this opportunity to thank all the researchers who have placed their trust in *BioMedInformatics* since its recent creation, as well as all the editors, reviewers and staff of *BioMedInformatics* who have made this success possible, which is not just a beginning, as the recent inclusion in SCOPUS shows.

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