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Combining Mechanistic Models and Machine Intelligence to Investigate the Druggable Region Surrounding the Fanconi Anaemia Pathway

Mohamed Alber *

Managing Editor, Journal of Space Exploration, Iraq

***Corresponding author:** Mohamed Alber, Managing Editor, Journal of Space Exploration, Iraq, E-mail: spaceexploration@scholarres.org

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Abstract

Given the imbalance between samples and candidate genes, and despite the amount of genomic data, it is challenging to develop predictive models that explain phenotypes as a function of gene expression or mutations. And in situations when sample availability is problematic, like in the case of uncommon diseases, this is more striking. Results we identified over 20 possible treatment targets by using multi-output regression machine learning approaches to estimate the potential impact of exogenous proteins over the signaling circuits that initiate Fanconi anemia-related cell functionalities. The systematic search for new targets in rare diseases is made possible by the use of artificial intelligence tools for the prediction of potentially causative links between proteins of interest and cell activities associated with disease-related phenotypes.

***Keywords:** Fanconi anaemia, Signaling pathways, Big data, Machine learning, Genomics*

Introduction

Genomic analysis is now a de facto Big Data discipline because to the sequencing technologies' incredibly quick increase in throughput over the past few years. Recent prospective studies have compared the generation of genomic data with other significant data generators like astronomy, Twitter, and YouTube and have come to the conclusion that genomics is either on par with or, possibly even more so than the Big Data domains considered in terms of data acquisition, storage, distribution, and analysis. Since machine learning techniques have lately been successfully applied to several areas of medicine, including radiology, pathology, ophthalmology, cardiology, etc., this appears to be the ideal situation for their use. In the case of human genomic data, however, the majority of applications have been unsupervised class discovery approaches, using gene expression data for visualization, clustering, and other tasks, primarily in single-cell or cancer. Supervised applications are limited to a few examples of relatively simple problems, in which a good balance between variables to predict and data available is satisfactory, such as inferring the expression of genes based on a representative sample. Therefore, despite the abundance of genetic data available, there aren't many translational applications because the most intriguing predictive scenarios have a major overfitting problem. The enormous number of variables (in the region of 20,000 genes), which poses a barrier to many traditional Machine Learning (ML) methodologies, makes it difficult to represent complex, multivariate phenotypes as a function of an undetermined number of genes. Therefore, new approaches that take advantage of the huge potential of ML applied to genomic Big Data are required to model diseases and find new treatments. An especially intriguing application of genetic data is in connection with the use of ML to model cell activity. These models provide a logical transition from genotype-level variants to phenotypic variations (at the scale of cells and

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organisms). The framework proposed is intriguing not only because it uses a causal link between genotype and phenotype but also because it is achieved with dimensionality reduction, despite the fact that these models are based on yeast, an organism much simpler than humans, and use yeast genomic data, which are much more abundant than human genomic data. In order to choose particular disease-related cellular mechanisms of interest, mechanistic models of human cell signaling or cell metabolism can offer the functional link between the available gene-level data (gene expression) and the cell phenotypic level. In fact, mechanistic models have aided in the understanding of disease mechanisms underlying various cancers, drug action mechanisms, and other biologically intriguing situations. For instance, molecular mechanisms that explain how stress-induced activation of brown adipose tissue prevents obesity, or the molecular mechanisms of death and the post-mortem ischemia of a tissue, are among the biologically interesting situations that these models have helped to illuminate. Actually, what we're going for here is drug repurposing, or finding new uses for medications already prescribed to treat other conditions. This is a great approach for rare diseases because it greatly speeds up the examination of potential compounds while also lowering the risk of failure. The problem of establishing links between potential proteins for a new indication and the FA hallmarks can be overcome with the right machine learning technique.

Conclusion

Our methodologies were insufficient from a microbiological standpoint to identify a high risk of infection or the transmission of bacteria that are resistant to antibiotics to crew members. However, we now view this risk as being incredibly low because to recent information from the ISS. Even though the risk was considered to be low, it became clear that microbial dynamics inside constrained and isolated ecosystems needed to be monitored in order to understand the effects of unique occurrences like the pollution brought on by the composting toilet. Additionally, baseline data on the microbiome of the habitat, its inhabitants, and post-sampling events would considerably enhance assessments of the effects of confinement on the inhabitants and the surfaces of the habitat. The majority of analogous research, whether they were conducted on the ground, like Mars500, or in space, like the ISS, revealed a similar picture of the long-term homogeneity, composition, and diversity of microbiomes.