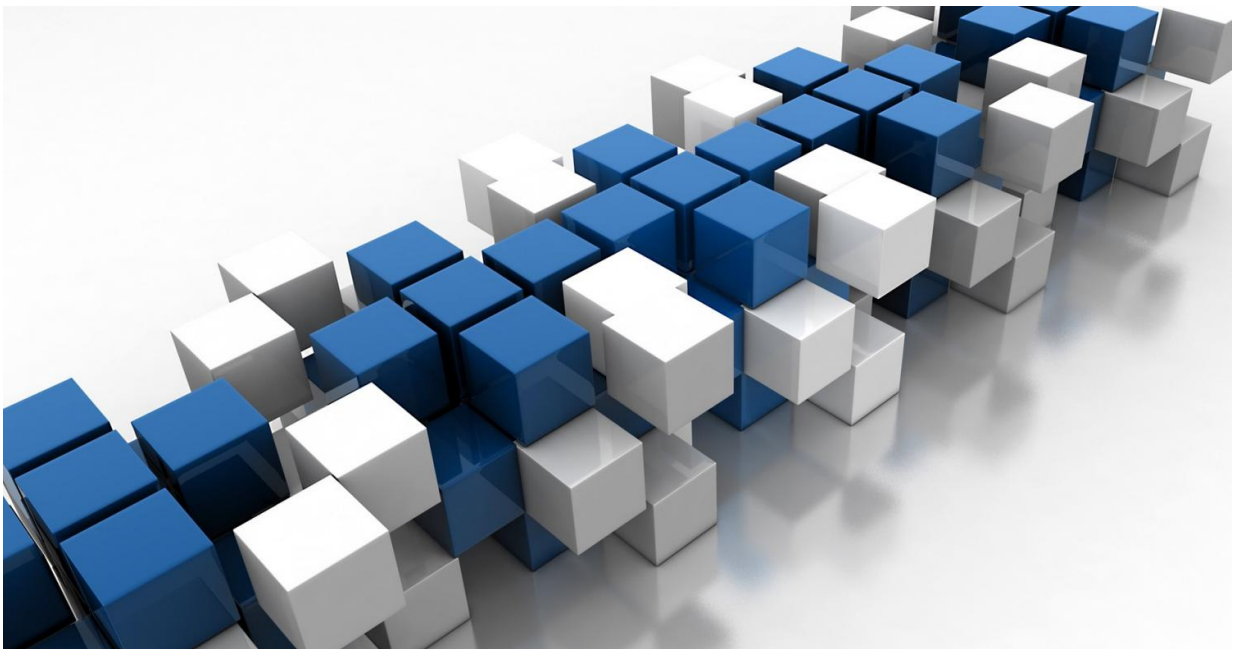


How artificial intelligence and machine learning will contribute to cancer patient care and vaccine design

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Artificial intelligence/machine learning involves the development of computer systems that perform tasks that would normally require human intelligence. AI/ML is used by people every day, for example, while using smart home devices or digital voice assistants. The use of AI/ML is also rapidly growing in biomedical research and health care. In a recent

viewpoint paper, investigators at Rutgers Cancer Institute of New Jersey and Rutgers New Jersey Medical School (NJMS) explored how AI/ML will complement existing approaches focused on genome-protein sequence information, including identifying mutations in human tumors.

Stephen K. Burley, MD, DPhil, and collaborators published the study December 2 in the *New England Journal of Medicine*.

What is the potential of AI/ML in cancer research and clinical practice?

We foresee that the most immediate applications of computed structure modeling will focus on point mutations detected in human tumors (germline or somatic). Computed structure models of frequently mutated oncoproteins (e.g., [epidermal growth factor receptor](#), EGFR, shown in Figure 2B of the paper) are already being used to help identify cancer-driver genes, enable therapeutics discovery, explain drug resistance, and inform treatment plans.

What are some of the biggest challenges for AI/ML in healthcare?

In the broadest terms, the essential challenges would likely include AI/ML research and development, technology validation, efficient/equitable deployment and coherent integration into the existing healthcare systems, and inherent issues related to the regulatory environment along with complex medical reimbursement issues.

How will this technology have an impact on vaccine design, especially with regard to SARS-CoV-2?

Going beyond 3D structure knowledge across entire proteomes (parts lists for biology and biomedicine), accurate computational modeling will enable analyses of clinically significant genetic changes manifest in 3D by individual proteins. For example, the SARS-CoV-2 delta variant of concern spike protein carries 13 amino changes. Experimentally determined 3D structures of SARS-CoV-2 spike protein variants bound to various antibodies, all available open access from the Protein Data Bank, can be used with computed structure models of new variant of concern spike proteins to understand the potential impact other amino acid changes. In currently ongoing work (as yet unpublished), we have used AI/ML approaches to understand the structure-function relationship of SARS-CoV-2 omicron variant of concern spike protein (with more than 30 amino acid changes), illustrating practical and immediate application of this emerging technology.

What is the next step to better utilizing AI/ML in cancer research?

Development and equitable dissemination of user-friendly tools that cancer biologists can use to understand the three-dimensional structures proteins implicated in human cancers and how somatic mutations affect structure and function leading to uncontrolled tumor cell proliferation.

More information: Stephen K. Burley et al, Predicting Proteome-Scale Protein Structure with Artificial Intelligence, *New England Journal of Medicine* (2021). [DOI: 10.1056/NEJMcibr2113027](https://doi.org/10.1056/NEJMcibr2113027)

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