ARIEL: Adversarial Neural Evolution for Unified Variant Forecasting and Proactive Therapeutic Design

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This research presents ARIEL, a deep-learning method for predicting COVID-19 variants and designing therapeutics to neutralize them. ARIEL is the first framework to simultaneously address these related problems of variant prediction and drug design. It does so through an AI-driven, adversarial evolution process. The COVID-19 spike protein is continually mutated to increase its own infectiousness, while the “inhibitor” (a protein that prevents infection) is continually mutated to decrease the virus’ infectiousness. Specifically, a Transformer-graph neural network pipeline (called “Dual Refinement” herein) first yields a numerical summary of the variant’s infectiousness given the corresponding inhibitor. Next, this output is used by two recurrent networks–trained via reinforcement learning–to design 1) a more infectious variant, and 2) a more effective inhibitor. This process is repeated continually until ARIEL produces a COVID-19 variant, plus an inhibitor tailored to neutralizing that variant. As assessed by the third-party benchmark SpikePro, 64 of 100 variants predicted by ARIEL are at least as infectious as the Delta variant. Similarly, as assessed by the third-party benchmark Rosetta, 84 of the corresponding 100 designed inhibitors are likely to bind to the virus, preventing infection. Furthermore, ARIEL was able to forecast Omicron’s spike mutations prior to Omicron’s November 2021 arrival. Not only does ARIEL predict (and rank) highly infectious variants and design reliable inhibitors, it does so several orders of magnitude faster than in-vitro methods. By predicting COVID-19 mutations and proactively designing therapeutic approaches to counteract them, ARIEL can help mitigate future variants even before they exist.

Awards Won:
Second Award of $2,000
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