Macro Roundup Article

Headline: Accurate Structure Prediction of Biomolecular Interactions With AlphaFold 3

Article Link: https://www.nature.com/articles/s41586-024-07487-w

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Tweet: .@GoogleDeepMind and @IsomorphicLabs announced AlphaFold 3, claiming a 50% accuracy improvement in the interaction between proteins, DNA, RNA, and other molecules. “We hope it will transform our understanding of the biological world and drug discovery.”

Summary: The introduction of AlphaFold 2 [July 2021] has spurred a revolution in modelling the structure of proteins and their interactions, enabling a huge range of applications in protein modelling and design. In this paper, we describe our AlphaFold 3 model with a substantially updated diffusion-based architecture, which is capable of joint structure prediction of complexes including proteins, nucleic acids, small molecules, ions, and modified residues. The new AlphaFold model demonstrates significantly improved accuracy over many previous specialised tools: far greater accuracy on protein-ligand interactions than state of the art docking tools, much higher accuracy on protein-nucleic acid interactions than nucleic-acid-specific predictors, and significantly higher antibody-antigen prediction accuracy. Together these results show that high accuracy modelling across biomolecular space is possible within a single unified deep learning framework.

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