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Transfer Learning for Protein Structure Classification at Low Resolution

Authors : Alexander Hudson, Shaogang Gong

Abstract : Structure determination is key to understanding protein function at a molecular level. Whilst significant advances have been made in predicting structure and function from amino acid sequence, researchers must still rely on expensive, time-consuming analytical methods to visualise detailed protein conformation. In this study, we demonstrate that it is possible to make accurate (≥80%) predictions of protein class and architecture from structures determined at low (>3A) resolution, using a deep convolutional neural network trained on high-resolution (≤3A) structures represented as 2D matrices. Thus, we provide proof of concept for high-speed, low-cost protein structure classification at low resolution, and a basis for extension to prediction of function. We investigate the impact of the input representation on classification performance, showing that side-chain information may not be necessary for fine-grained structure predictions. Finally, we confirm that high resolution, low-resolution and NMR-determined structures inhabit a common feature space, and thus provide a theoretical foundation for boosting with single-image super-resolution.

Keywords : transfer learning, protein distance maps, protein structure classification, neural networks
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