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Improved Protein Contact Predictions using Diverse Neural Networks WENDY BILLINGS, DENNIS DELLA CORTE, Brigham Young University — Substantial progress has been made toward the accurate prediction of protein tertiary structure from primary sequence, aided by machine learning. Current success is based on two-stage protocols: first, prediction of macromolecular structure restraints by deep convolutional neural networks; second, application of these restraints to construct a folded three-dimensional structure of the target protein. Accuracy of the final atomic model depends heavily on the individual quality of both stages. Here we evaluate inter-residue distance predictions made by neural networks in the first stage by way of the related contact prediction task. Using published protein structures from CASP13, we calculate the contact prediction performance of several networks (including AlphaFold, trRosetta, and our own ProSPr) both individually and combined in ensembles. Our results demonstrate that combining the predictions of diverse neural networks can improve contact prediction accuracy and outperform the best individual networks. We call for increased availability of distance prediction networks for a community-based ensemble approach to superior protein contact prediction.

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