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Protein Structure Prediction Using 3-D ResNet[1] BRYCE HEDELIUS, Brigham Young University — Predicting a protein's structure from its amino acid sequence is a longstanding problem. Deep learning methods based currently produce the best predictions. Sequence alignments are used to generate features, such as amino acid identity and propensity. A network then predicts characteristics of the structure such as inter-residual distances or torsion angles which are used to generate a prediction of the structure. Here I propose a method based on a 3D residual neural network. The features are derived from a generalized Potts model that considers three-wise interactions and the labels include planar and dihedral angles involving three residues. The predictions will then be used as constraints in a molecular dynamics simulation. Higher order constraints are expected to aid structure generation while improving predictions of other constraints.

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