Background

Why proteins? - Proteins underpin every aspect of biological activity

The properties of a protein, and its biological functions, are highly dependent of its 3D structure. X-ray crystallography and nuclear magnetic resonance are the main approaches for experimental determination of tertiary structures. However, as the techniques for primary structure determination have become more effective and sequence and structure databases have grown, so has the possibility for computational predictions of protein folding. Even a low-resolution model, only showing residue positions, can be useful. Kihara et al. (2009) states that the major reason for not applying predictions in practical work is that the quality of the model is unknown, not that it is inaccurate. Even somewhat inaccurate models, or models with low resolution, can be used in for example early stages of drug development, as long as the estimated error is known, entailing high accuracy model quality assessments for ranking predicted models. [1]

Protein structure and folding

Protein structure prediction

Model Quality Assessment

Deep learning

3DCNN