https://www.nature.com/articles/s41586-019-1923-7.epdf?author_access_token=Z_KaZKDqtKzbE7Wd5HtwI9RgN0jA1PrccXfIbc6e-tGSgazNL_XdtQzn1PHfy21qdcxV7Pw-k3htw%3D%3D

AlphaFold is Google DeepMind's protein structure prediction software that uses deep learning to minimize energy potential by modifying torsion angles.

AlphaFold's primary component is a CNN trained off of protein samples to predict distances between atoms within pairs of residues of a protein. Given an amino acid sequence, it produces a discrete probability distribution for every residue pair within a 64 by 64 area in the distance matrix. These local predictions can be combined to create a full set of predictions and a distance histogram (a matrix view of the distances between any two residues). *SIDENOTE: Network also outputs confidence for each prediction*

Proteins were parameterized via torsion angles of each residue the coordinates for structure were generated via "differential models of protein geometry".

1 | Hyperparameters/Details

- Dropout (keep prob 0.85)
- Parallelized SGD (batch sz 4)
- Activation function: ELU
- Learning rate: 0.06
- Learning rate decay (halved at 150000, 200000, 250000, 350000 steps)
- 5 days training time