**AlphaFold 2**

- Protein sequence, length = L
  - MLIGAWS...

**Homologous sequence**
- Related by evolution

PSSM: position specific scoring matrix

MSA: multiple sequence alignment
1. Query the seq DB
2. Extract similar sequences
3. MSA
4. PSSM
   - \( \rightarrow \) MLIGAWSPIW
   - \( \rightarrow \) MLGAPIPSTW
   - \( \rightarrow \) MLGAWP
   - \( \rightarrow \) MLGESWSPIAW

**CASP 15**
- Critical Assessment of Structure Prediction (CASP 15)
- FM
- TBM
- Free modeling
- Template-based modeling

**PDB**
- Protein data bank
- \( \sim \) 20k structures
- Unique sequence database
- \( \sim \) 10k sequences

**MSA**
- Weighted variant LCS
- (longer common subsequence)

**Profile PSSM**
- MSA
\[
\begin{align*}
\mathbf{f}_i &\in \mathbb{R}^{45} \quad \forall i = 1 \ldots L \\
\mathbf{f}_{ij} &\in \mathbb{R}^{45} \quad \forall i,j = 1 \ldots L
\end{align*}
\]

\[
\mathbf{F}_{ij} = \text{feature vector for } (i,j) \text{ cell}, \quad \text{extra!}
\]

\[
\begin{bmatrix}
\ell_i \\
\ell_j \\
\mathbf{f}_{ij}
\end{bmatrix}
\]

\[
\text{G-coefficient vector}
\]

\[
\mathbf{f}_i = \begin{bmatrix}
\ell_i \\
\mathbf{1}_{45} \\
\mathbf{1}_{45} \\
\mathbf{1}_{45} \\
\mathbf{1}_{45} \\
\mathbf{1}_{45}
\end{bmatrix}
\]

\[
145 \text{ dim features!}
\]
Choose starting \( ij \) within first \( 6 \times 6 \) crop

\( L = 520 \)

Use padding \( @52 \) at around

For some protein

\( \leq \) multiple crops with \( ij \) starting + slide
The diagram shows a series of transformations and operations on data with dimensions and channels. The operations include projection, convolution, and pooling. The text describes the process in detail, mentioning input channels, convolutional layers, and output dimensions. The diagram illustrates the flow of data through these operations.
Dilate $\oplus$ ($d$ = dilation)

$3 \times 3$ dilation

d = 1

d = 2

d = 4
22x dilation there!

Predicted logits

Out-Channels = 64

64 bins for distance prediction

CE-vink loss (dim=2)

for softmax

two distance bins

\[ 2a = 22A \]

divide into 64 bins

\[ \frac{22A}{64} \]