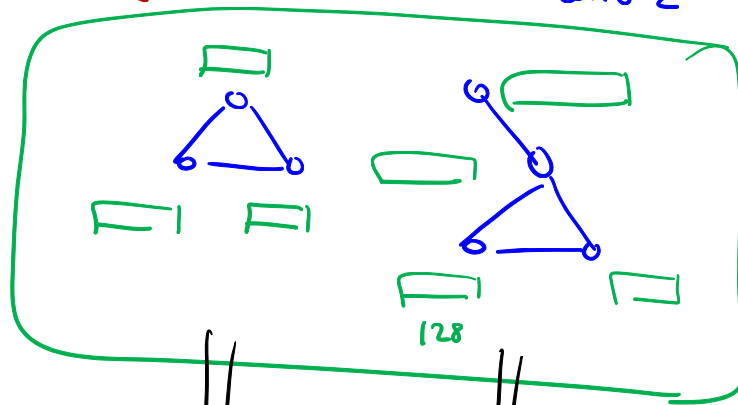
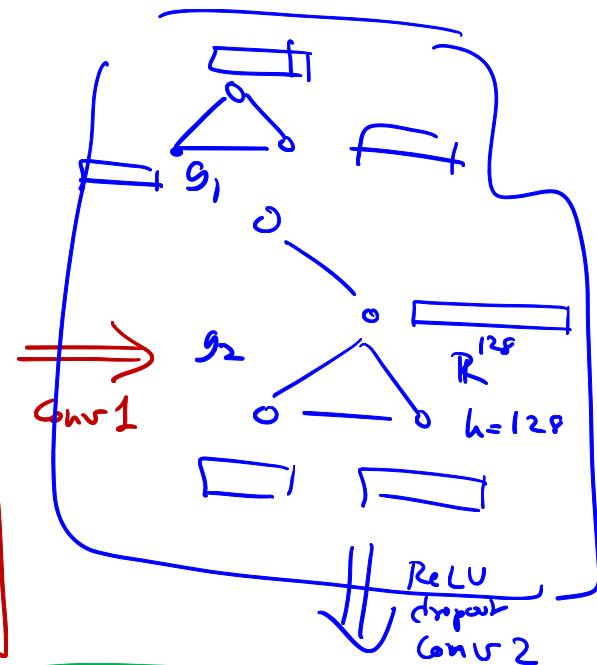


batched graph  
batch size = 2



Conv layers = 2

$$h = \text{Conv1}(g, \text{in-feat})$$

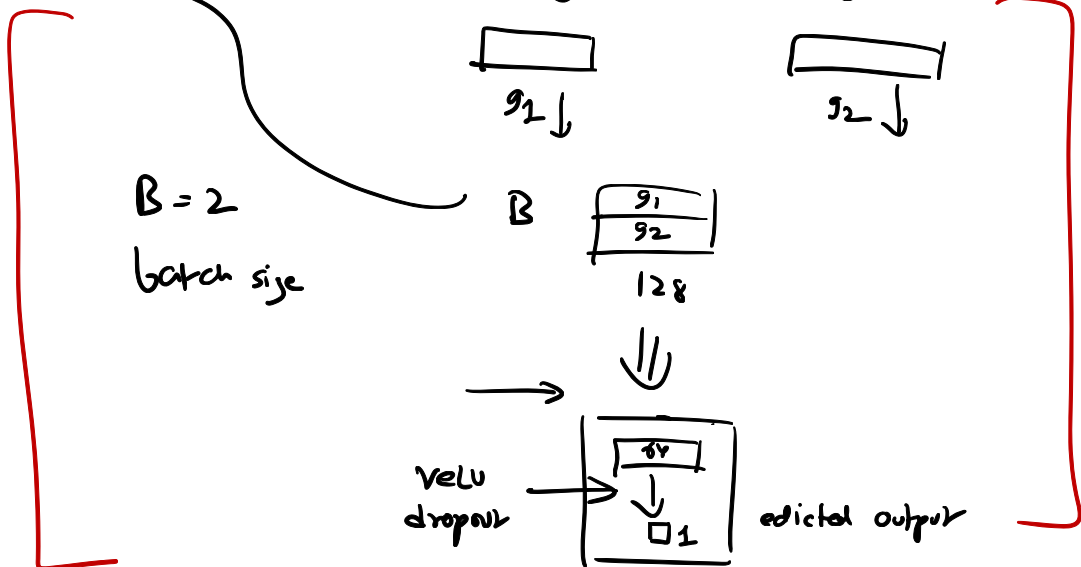
$$h = \text{Conv2}(g, h)$$

pooling readout

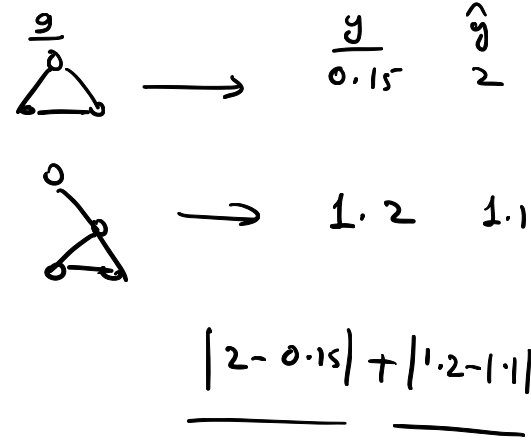
$$x = \text{readout}(g, h)$$

$$h = N \times 128$$

N: # of nodes in batched graph



loss: Regression  
 ↓  
 MSE ~~loss~~  
 Mean Squared Error



L1 loss: MAE  
 Mean Absolute Error

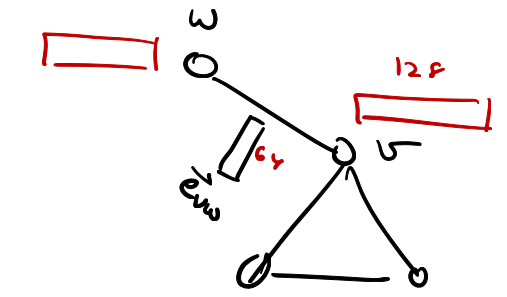
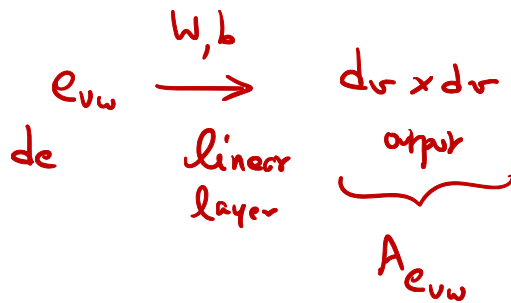
MPNN: Message Passing NN

$$M_v^{t+1} = \sum_{w \in N(v)} M_t^w (h_v^t, h_w^t, e_{vw})$$

$$h_v^{t+1} = U_t (h_v^t, M_v^{t+1})$$

$e_{vw} \rightarrow$   
 $d_e$ : hidden dimensionality = 64

$h_v$ :  $d_v = 128$  dim



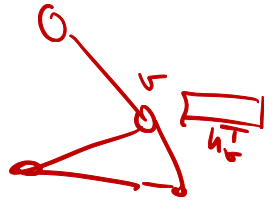
$$M_t^w = \left( \underbrace{A_{e_{vw}}}_{128 \times 128} \cdot \underbrace{h_w^t}_{128 \times 1} \right)_{128 \times 1}$$

$U_t$ : GRU (gate recurrent unit)

Simplified version of LSTM

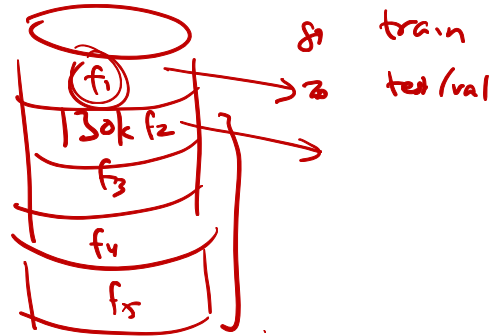
last hidden state  $h_s^T \forall v \in g.$

$T$ : # of update steps!



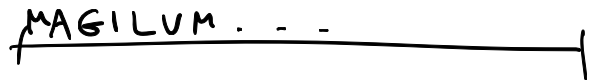
$S$  random splits

$S - CV$



Protein structure

1) Primary (sequence of AA)



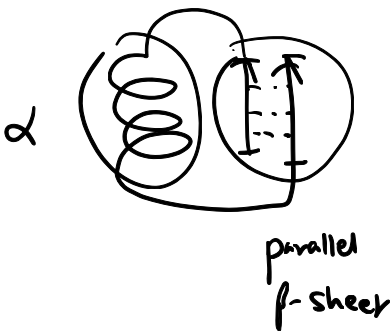
2) Secondary structure (Elements)

local structure

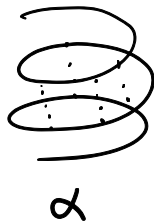
$\alpha$ -helix

$\beta$ -strands/sheets

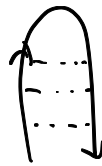
loops



parallel  $\beta$ -sheet



$\alpha$

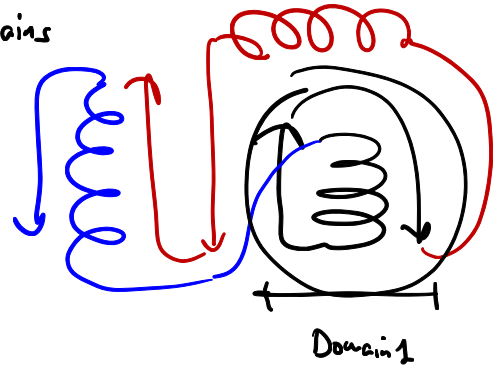
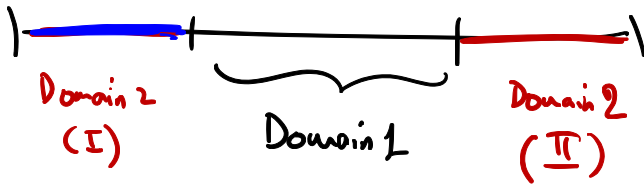


anti parallel  $\beta$



### 3) tertiary (3D) structure ←

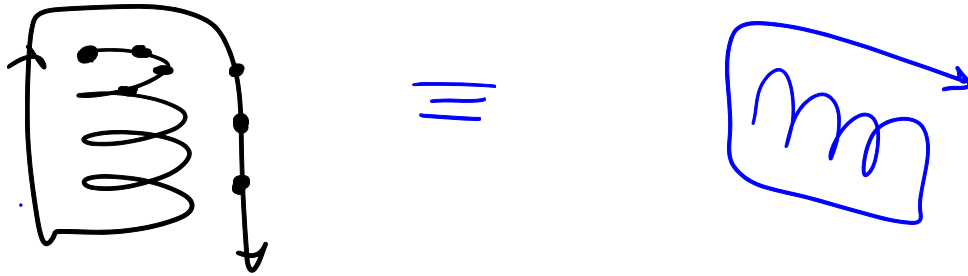
whole chain → Domains



### 4) Quaternary structure

multiple-chains for a Complex

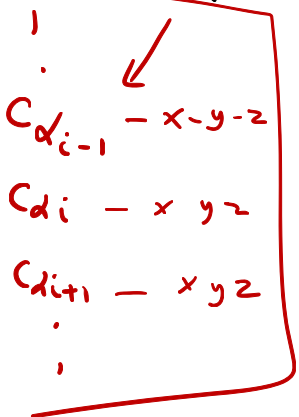
how to compare true & predicted structure



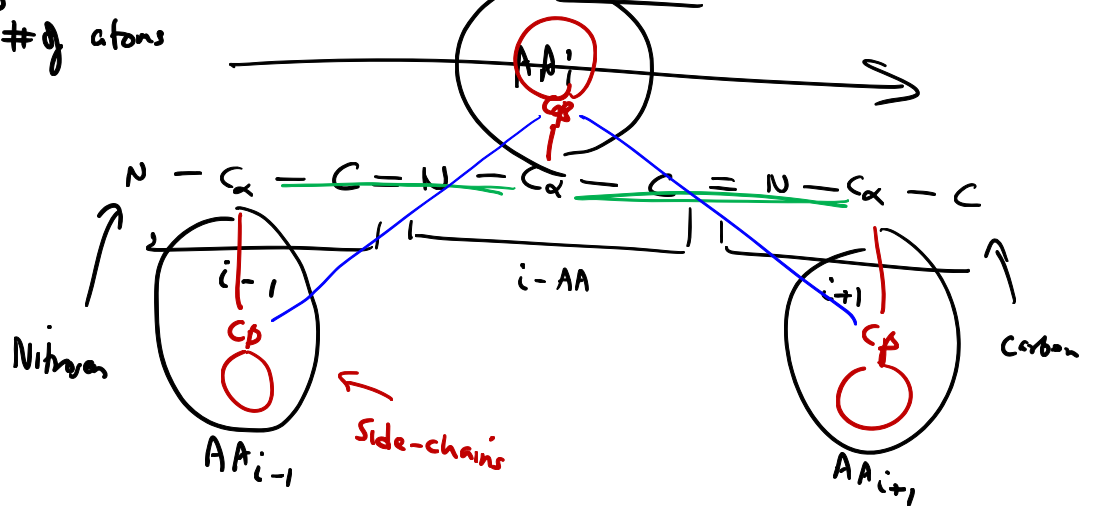
N: length N

# of AA → # of atoms

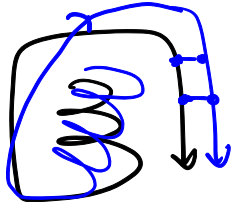
$C_{\alpha}$  → Cp



Backbone chain (AA)



# Super position



→ RMSD : root mean sq  
distance

→ distance RMSD (pair-wise)