Capstone Project

I. Milestone 1: 11th Apr, midnight

send group info before midnight

Alphafold 2

target : Nres x 21

Msa_feat : N_{clust} x Nres x 21 (pssm)

residue_index : pos info Nres

Nres : protein length

Natoms : all atoms

C_α : x, y, z

output

Pair I : input

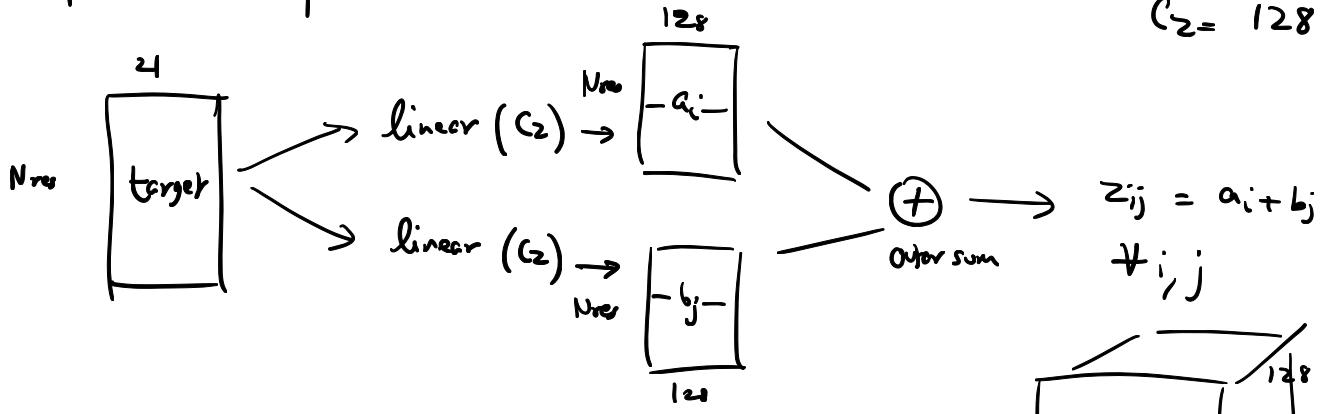
template_pair (3D similar structure)

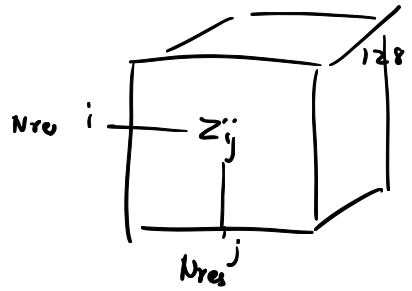
template angle

we don't have in sidechainnet.

raw input → processed inputs

$C_2 = 128$





pair-representation

$z_{ij} = z_{ij} + p_{ij}$ final pair-wise rep

$d_{ij} = (idx_i - idx_j)$

bin into $[-32, -31, \ldots, 31, 32]$

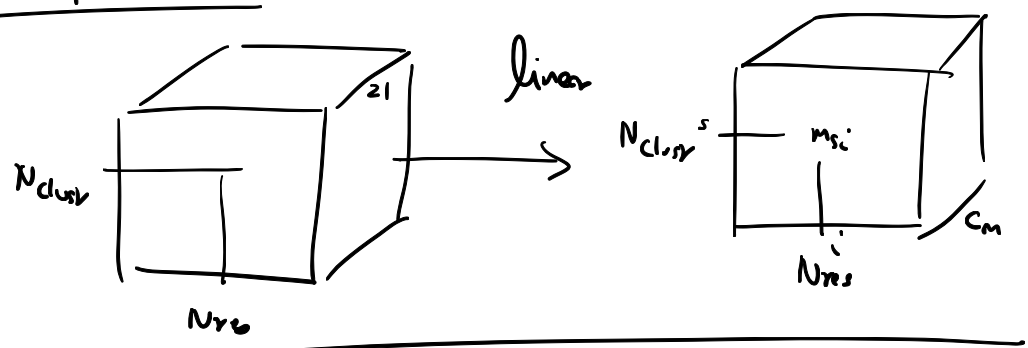
one-hot

p_{ij} = linear (one-hot (d_{ij}))

← relative position module

$p_{ij} \in \mathbb{R}^{C_2} \equiv \mathbb{R}^{128}$

msa_representation

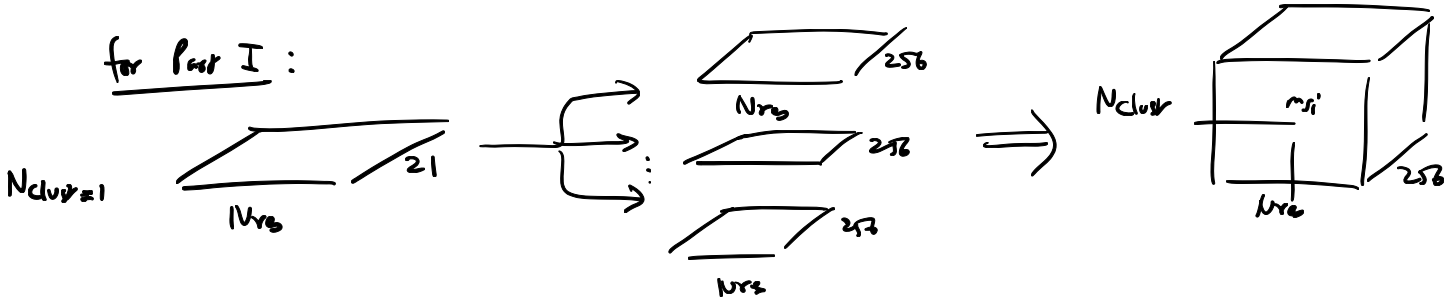


$c_m = 256$

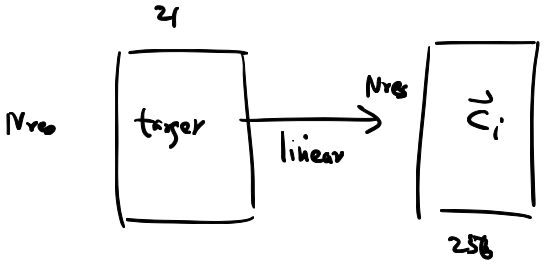
$\vec{m}_{si} \in \mathbb{R}^{256}$

actual Alphafold

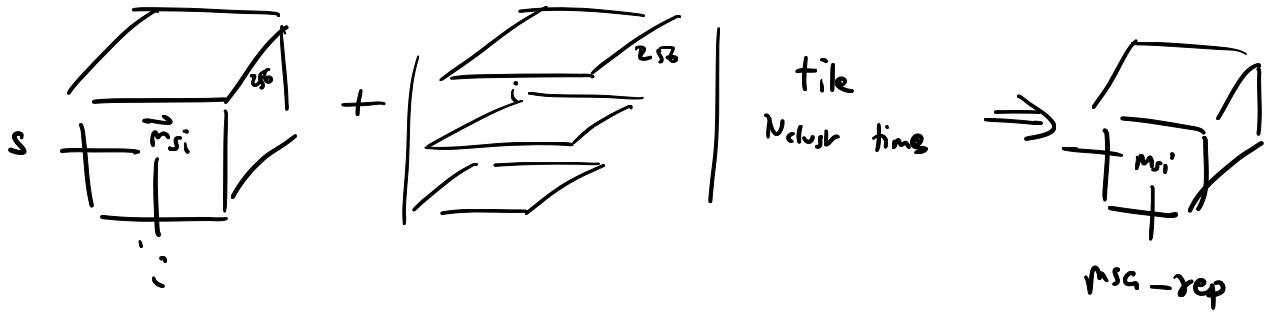
for Part I:



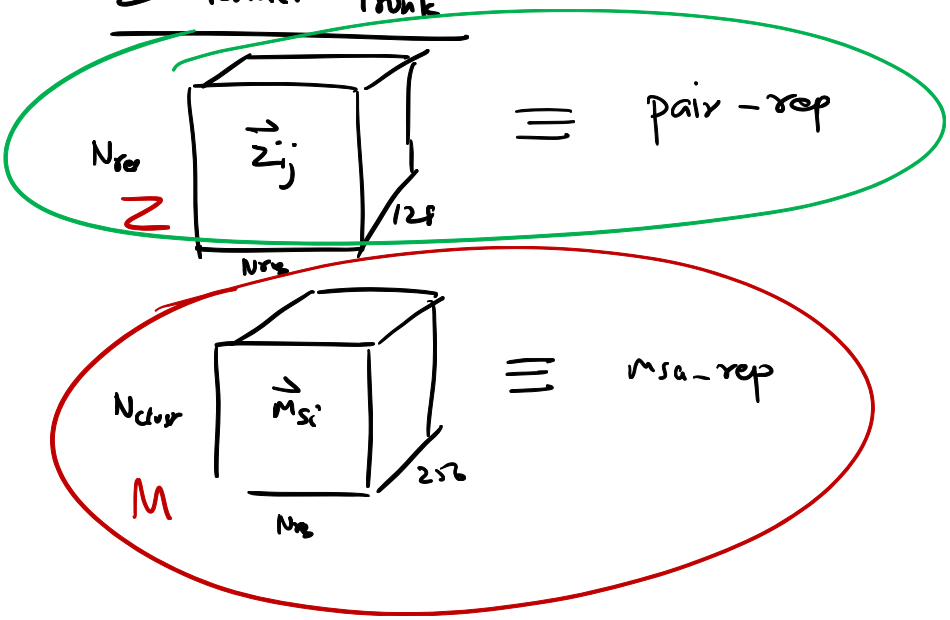
N_{clust} linear layers!



$$m_{si} = \vec{m}_{si} + \vec{c}_i$$



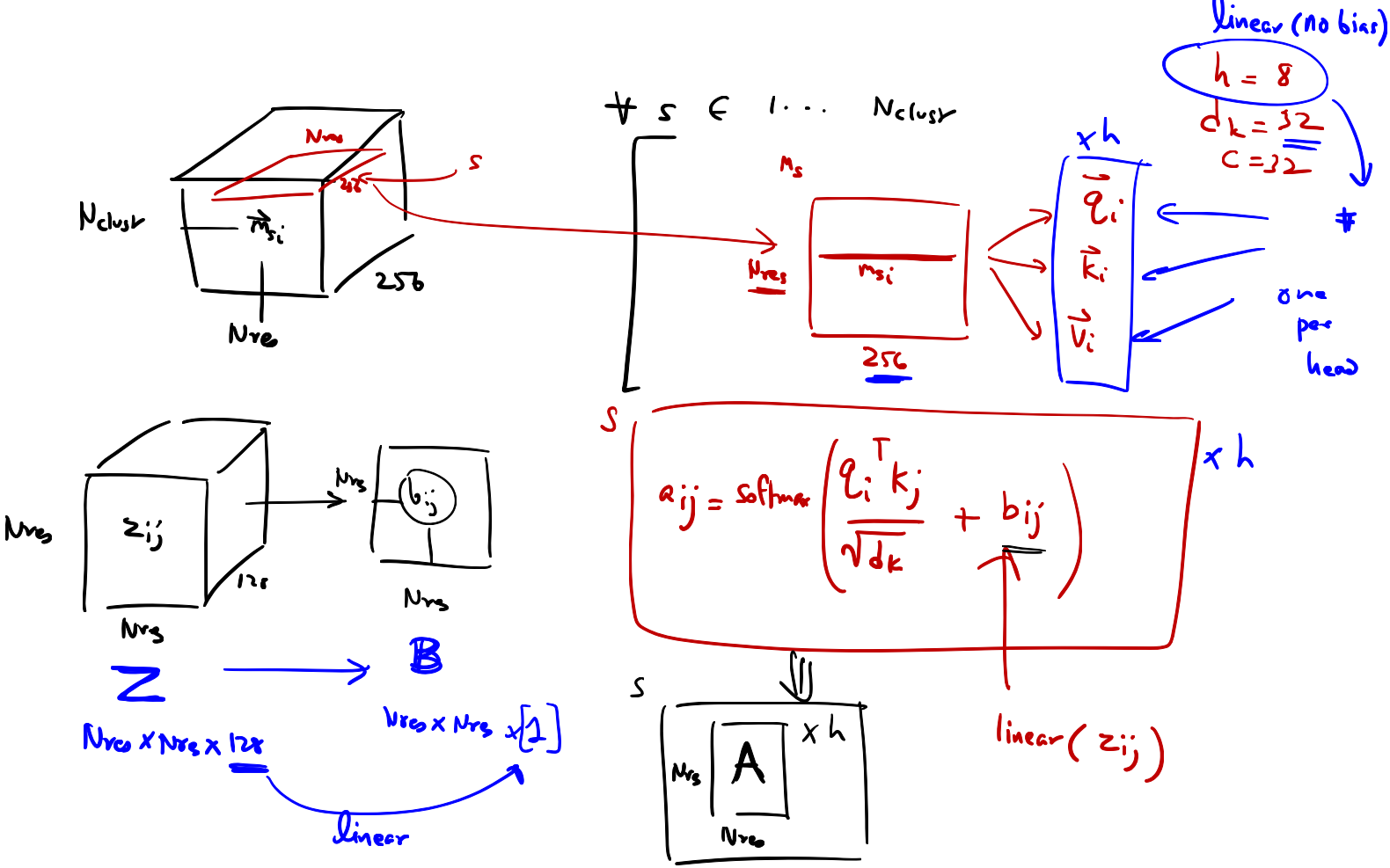
Evoformer Trunk

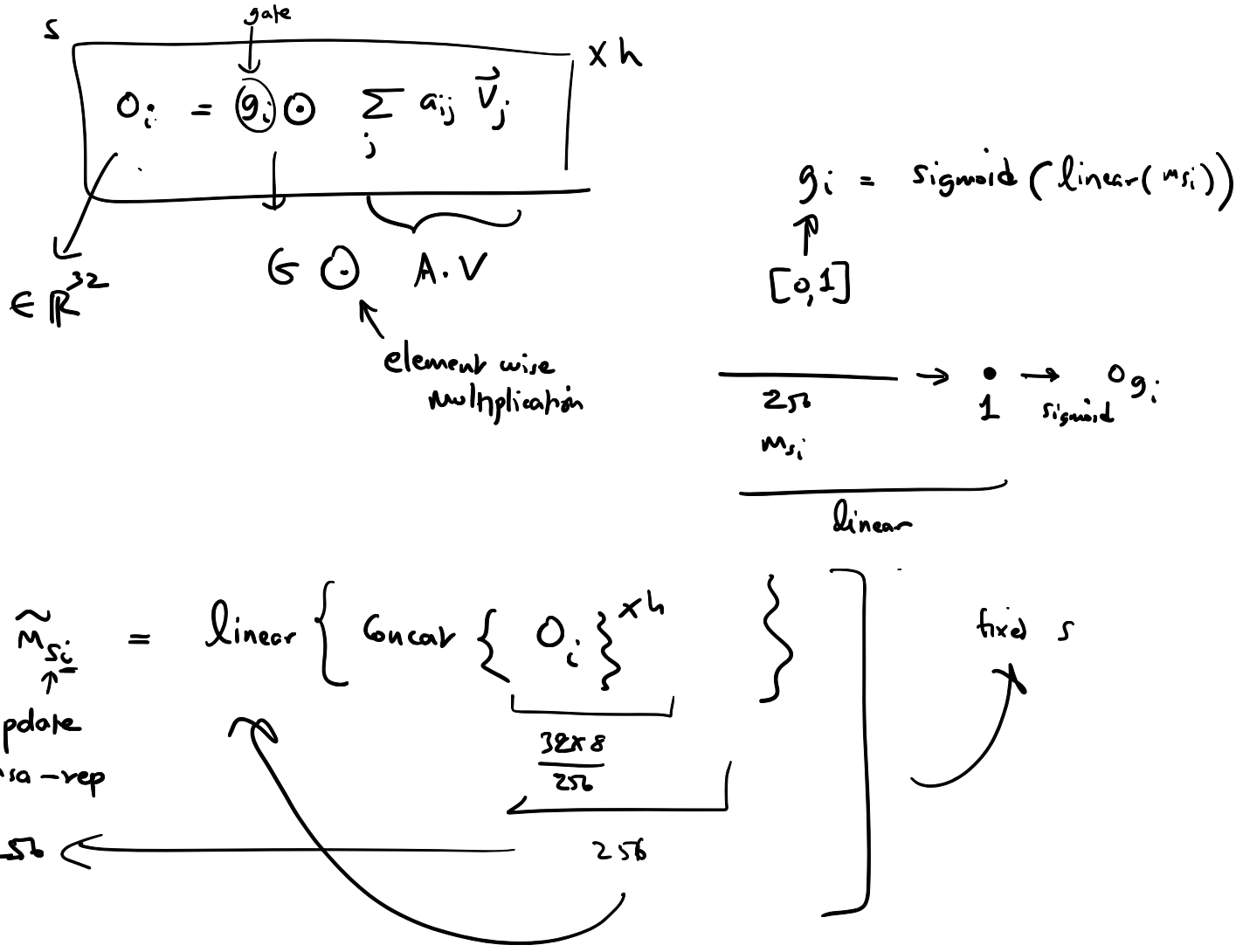


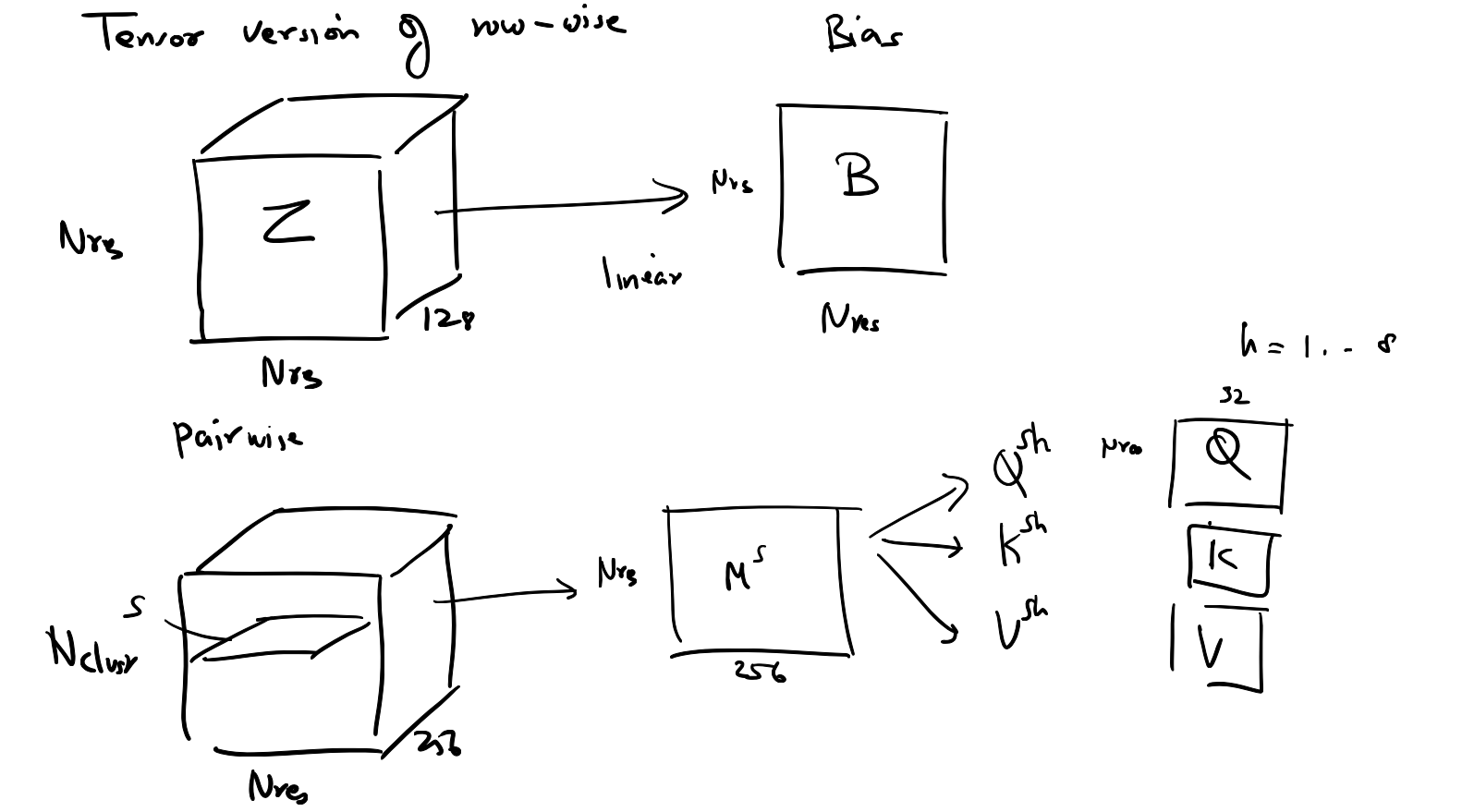
triangular attention
multiplicative attention

axial attention
↙
row & col : alternating

I. row wise attention (gated, pair bias)




s
gate
x h
$O_i = g_i \odot \sum_j a_{ij} \vec{V}_j$
$\in \mathbb{R}^{32}$
G ⊙ A.V
element wise multiplication
g_i = sigmoid (linear(m_{si}))
[0,1]
256
1
sigmoid
m_{si}
linear
$\tilde{m}_{si}$ = linear { Concat { O_i }^{x h} }
fixed s
Update msa-rep
32x8
256
256
$\mathbb{R}^{256}$


Tensor version of row-wise
Bias
Nres
Z
128
Nres
Nres
linear
Nres
B
Nres
pairwise
h = 1 .. 8
32
Q^{sh}
K^{sh}
V^{sh}
Nres
Q
K
V
s
Nclust
Nres
256
Nres
M^s
256

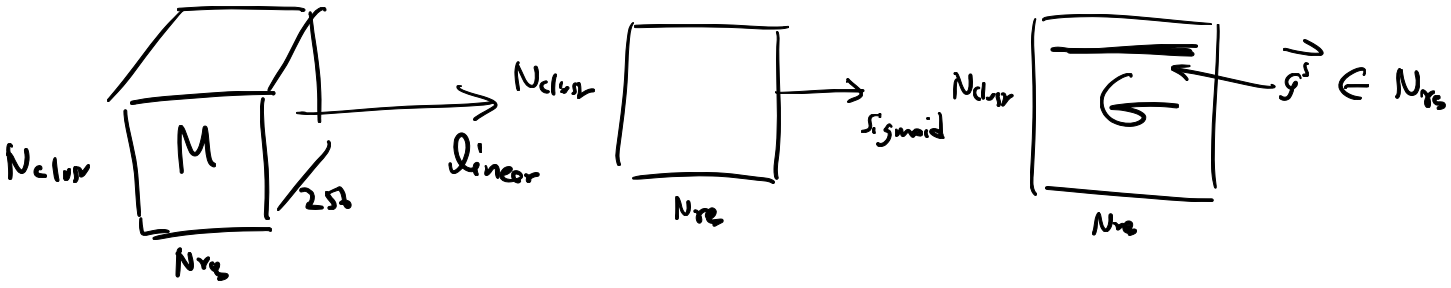
$$A^{sh} = \text{softmax}_{\text{over rows}}\left(\frac{Q^{sh}(K^{sh})^T}{\sqrt{d_k}} + B\right)$$

$Q^{sh}: (N_{res} \times 32)\ (32 \times N_{res})$ $\quad (K^{sh})^T$

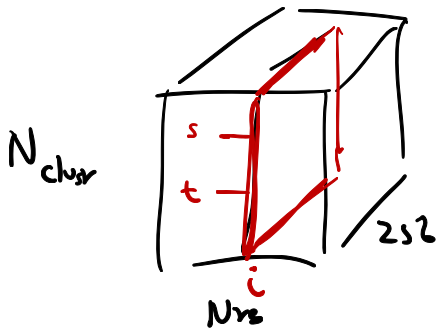
$N_{res} \times N_{res}$

$$O^{sh} = \vec{g}^{s} \odot (A^{sh} \cdot V^{sh}) \qquad N_{res} \times 32$$

$$M^{s} = \text{linear}\left(\underset{h}{\text{Concat}}\{O^{sh}\}\right)$$

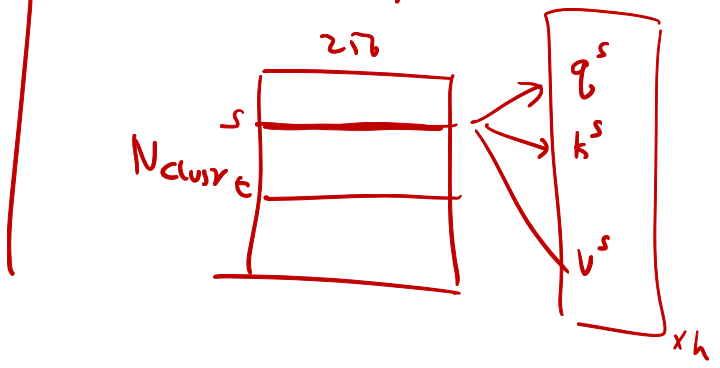


II. Col-wise attention (gated)



$\forall i = 1 \dots N_{res}$

attention over sequence in N_{clust}



$C = 32$

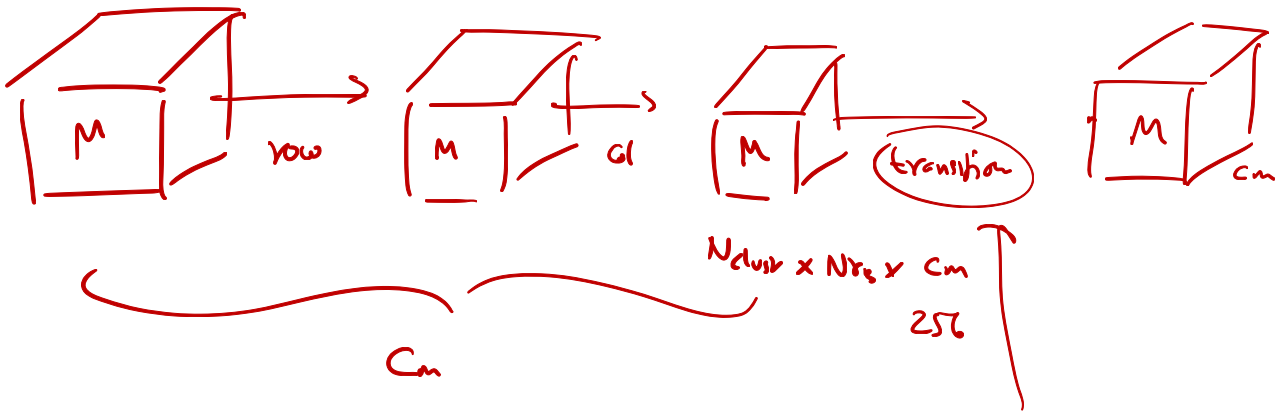
Proj dim

$h = 8$

$$\left[a_{st} = \text{Softmax}\left(\frac{q^s \cdot k^t}{\sqrt{c}} \right) \right]^{x\,h}$$

$$\left[o_s = g_s \odot \sum_t a_{st} \cdot \vec{v}_t \right]_{x\,h}$$

$$\tilde{m}_{si} = \text{linear}\left(\text{concat}\left\{ o_s \right\}^{x\,h} \right)$$



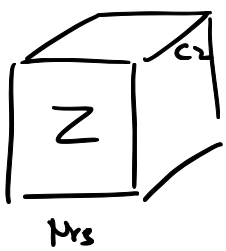
III

transition : 

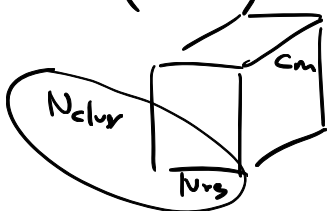
linear ($c_m \rightarrow 4c_m$)

linear ($4c_m \rightarrow c_m$) ←

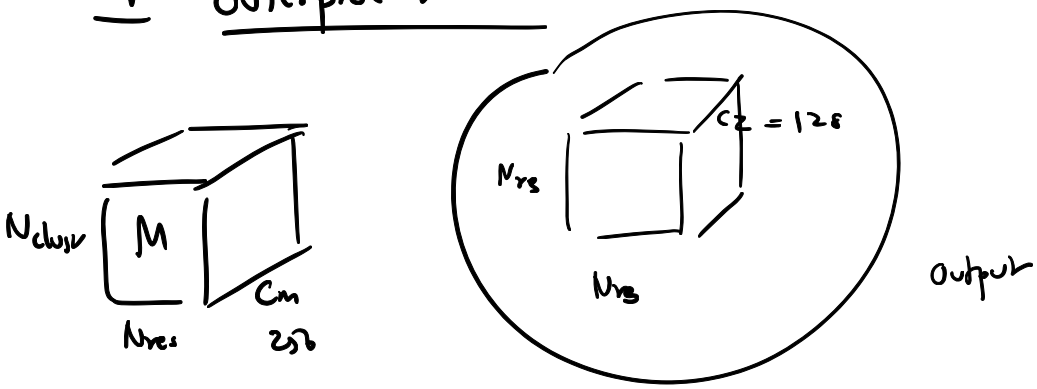
$C_2 = 128$

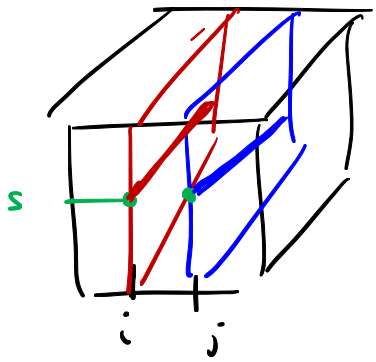
N_{rs} 

+ Outer product mean (M)



IV Outerproduct mean





$C = 32$ $\quad C_M$

$$\vec{a}_{si} = \text{linear}(\vec{M}_{si})$$

$$\vec{b}_{si} = \text{linear}(\vec{M}_{si})$$

Standard vector outer product

$$O^s_{ij} = \vec{a}_{si} \otimes \vec{b}_{sj} \longrightarrow C \times C$$

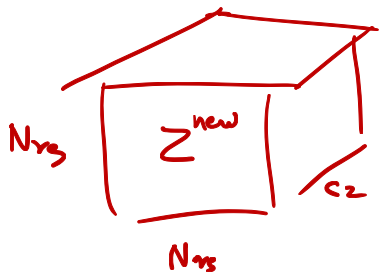
$$O_{ij} = \underset{s}{\text{mean}} \{ O^s_{ij} \} \quad C \times C \xrightarrow[\text{flatten}]{} C \cdot C$$

$C = 32$

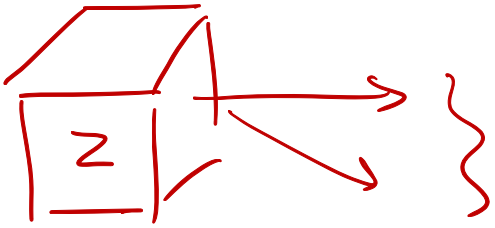
$$z_{ij} = \text{linear}\{O_{ij}\}$$

$C_Z = 128$

new Z tensor



$$Z = Z + Z^{new}$$



triangular & multiplicative attn.