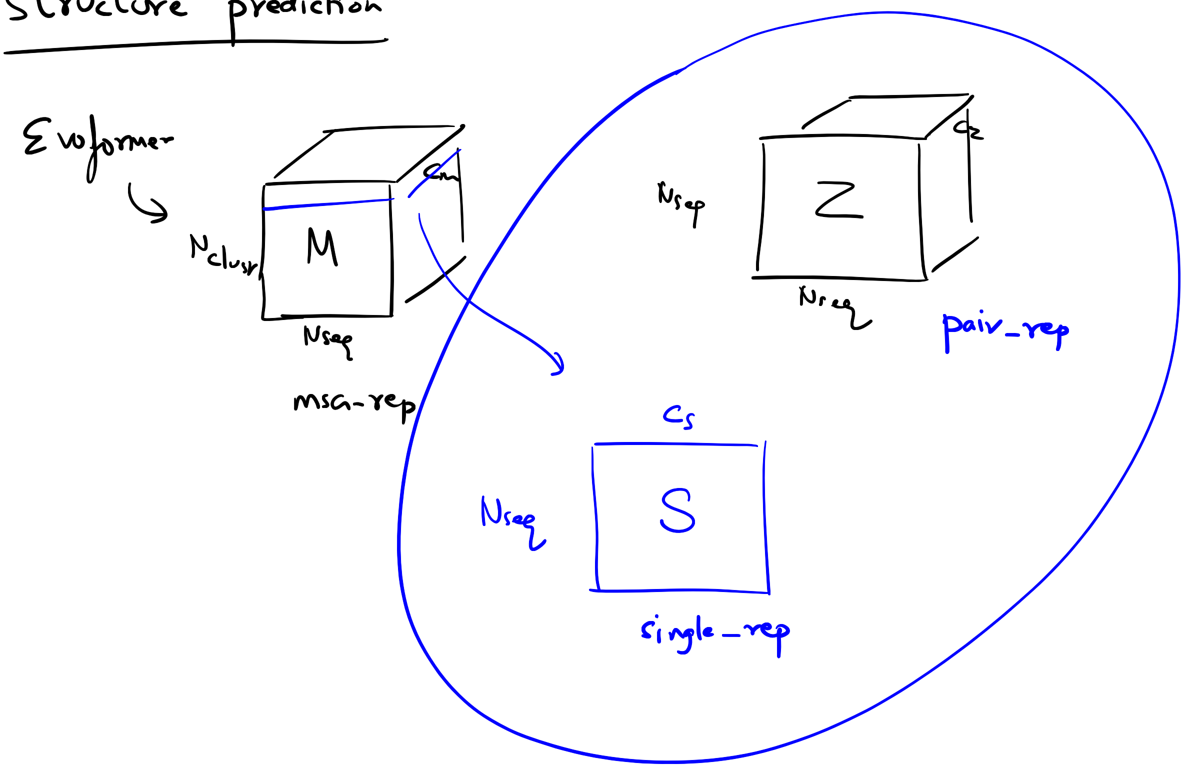
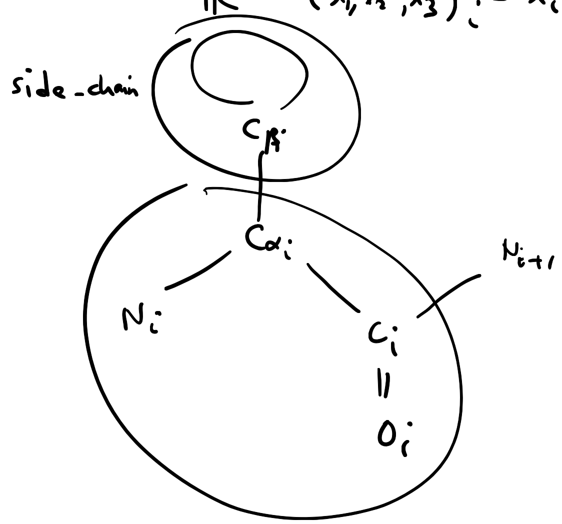
structure prediction

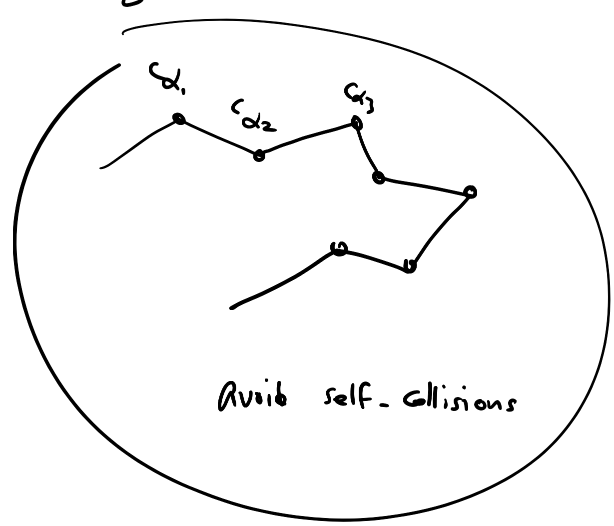


Predict C_α co-ordinate $\forall$ for $i = 1, \dots, N_{seq}$

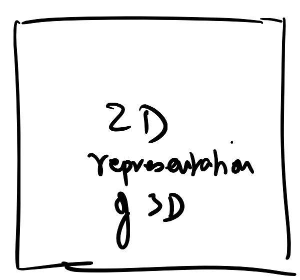
$\mathbb{R}^3 \quad (x_1, x_2, x_3)_i = \vec{x}_i$



Per residue



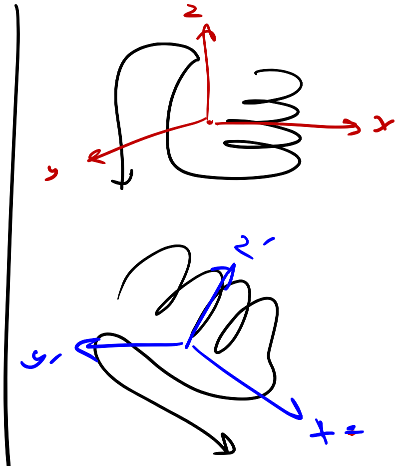
distance map

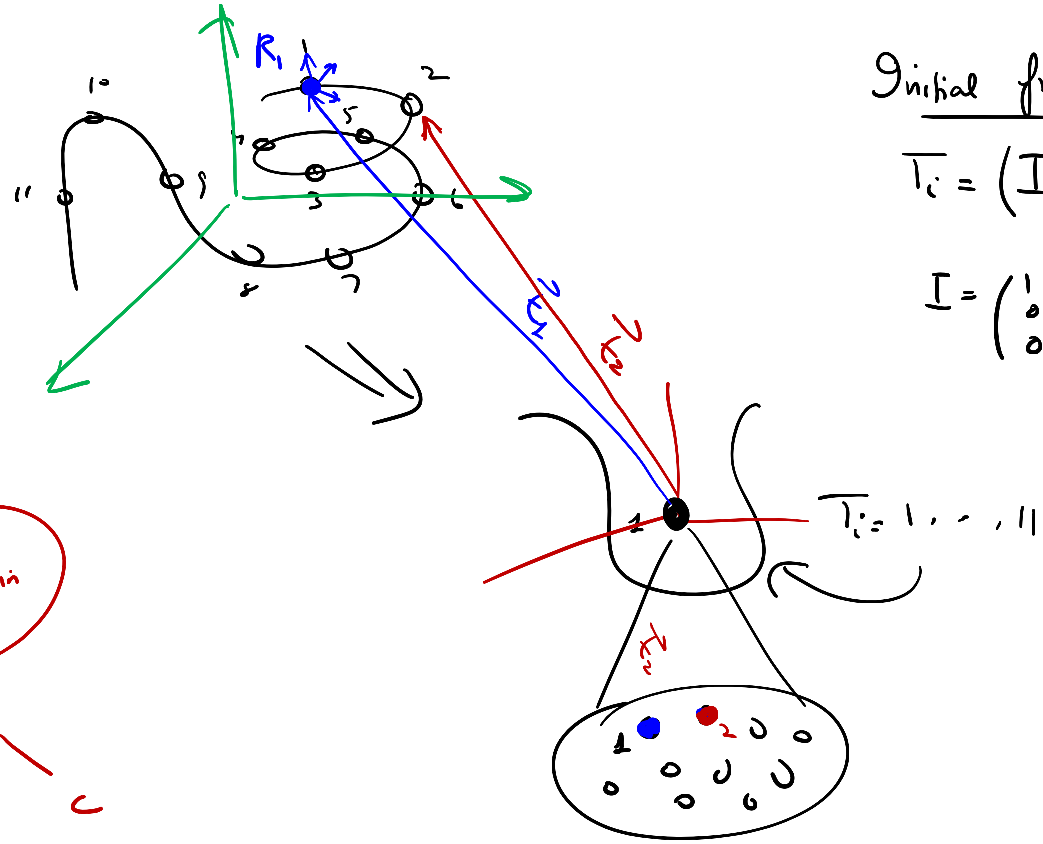


$d_{ij} = \|\vec{x}_i - \vec{x}_j\|$

local reference frame per atom

$$\underbrace{T_i}_{\text{frame}} = (\underbrace{R_i}_{\substack{\text{rotation matrix} \\ \mathbb{R}^{3\times 3}}}, \underbrace{\vec{t}_i}_{\substack{\text{translation vector} \\ \mathbb{R}^{3}}})$$

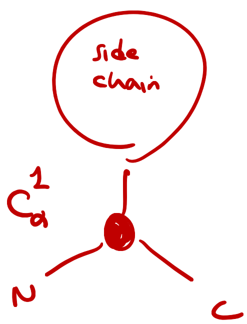




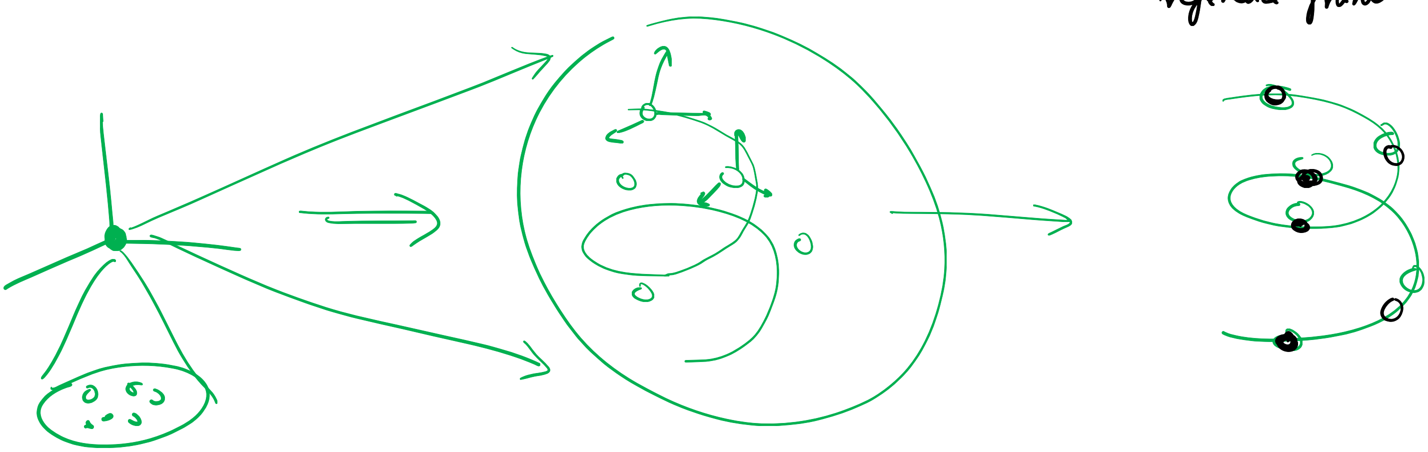
Initial frames

$$T_i = (I, \vec{0})$$

$$I = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \vec{0} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

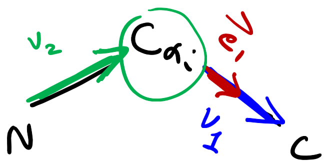


T_i : mapping from local reference frame to the global reference frame



true frame $\qquad$ predicted frame

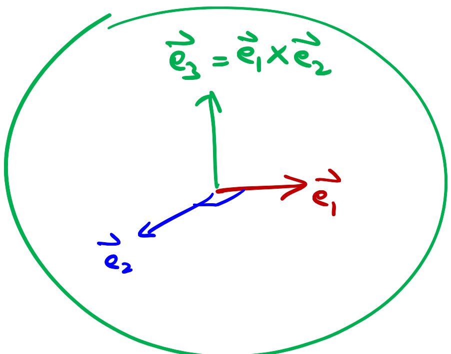
T_i^{true} $\qquad$ T_i



$\vec{v}_1 = \vec{C} - \vec{C}_{\alpha_i}$

$\begin{pmatrix} x \\ y \\ z \end{pmatrix} \qquad \begin{pmatrix} x \\ y \\ z \end{pmatrix}$

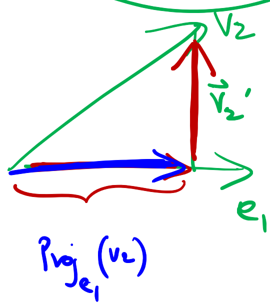
$R_i^{true} \equiv$



$\vec{t}_i^{\,true} = \vec{C}_{\alpha_i}$

$\vec{e}_1 = \dfrac{\vec{v}_1}{\|\vec{v}_1\|}$

$\vec{v}_2 = \vec{C}_{\alpha_i} - \vec{N}$



$\vec{v}_2{}' = \vec{v}_2 - \underline{\underline{\mathrm{Proj}_{\vec{e}_1}(v_2)}}$

Orthogonal

$= \vec{v}_2 - (\vec{e}_1^{\,T}\vec{v}_2)\vec{e}_1$

$\vec{e}_2 = \dfrac{\vec{v}_2{}'}{\|\vec{v}_2{}'\|}$

$\vec{e}_3 = \vec{e}_1 \times \vec{e}_2$

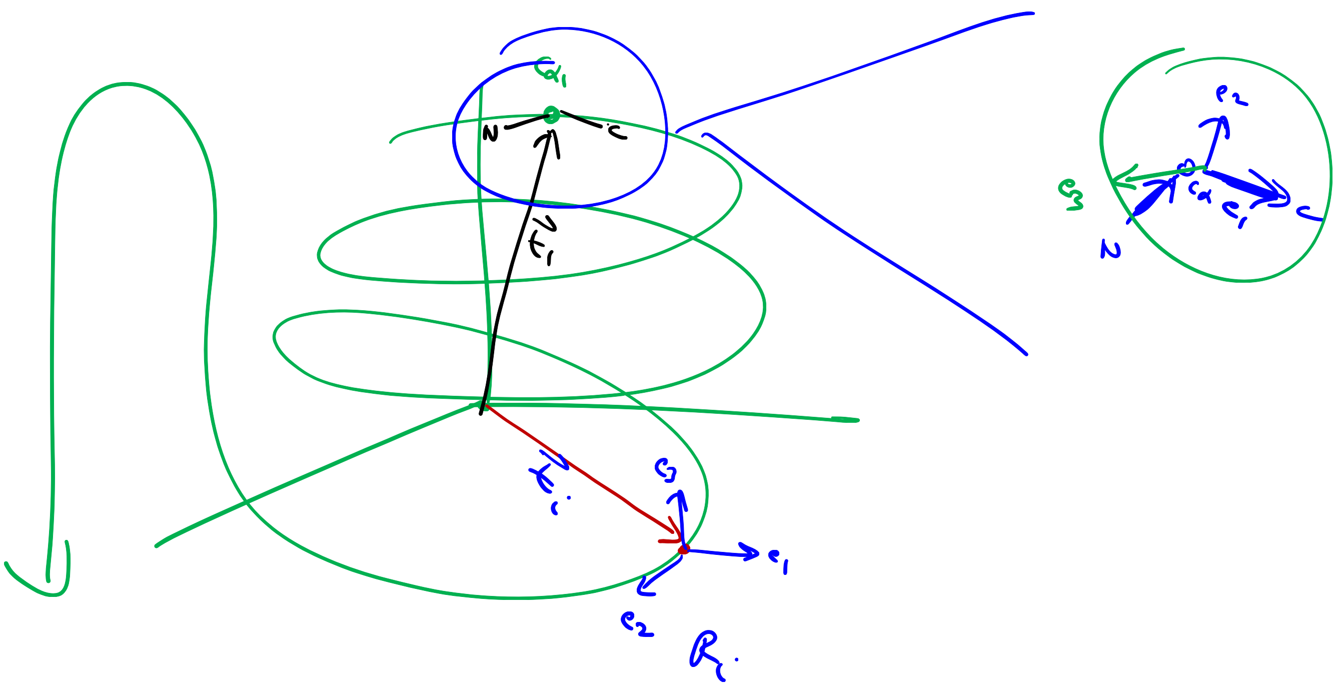
$$= \begin{array}{c} \\ \vec{e}_1 \\ \vec{e}_2 \end{array} \begin{vmatrix} i & j & k \\ e_{11} & e_{12} & e_{13} \\ e_{21} & e_{22} & e_{23} \end{vmatrix}$$

$$= i\,\underbrace{(e_{12} \cdot e_{23} - e_{13} \cdot e_{22})}_{e_{31}} - j\,(e_{11} \cdot e_{23} - e_{13} \cdot e_{21})$$

e_{32}

$$+ k(\underbrace{e_{11} e_{22} - e_{12} e_{21}}_{e_{33}})$$

$$\vec{e}_3 = (e_{31}, e_{32}, e_{33})$$



$\overline{T_i}^{true}$ $\forall\, C\alpha_i$ (actually all atoms)

$$T_i = (R_i, \vec{t}_i) = (I, \vec{\emptyset}) \quad \forall\, i = 1 \ldots N_{Res} \quad (C\alpha_i)$$

focus on

for $l = 1 \ldots 8$

$s_i = \text{IPA}(s_i) + s_i \quad \forall\, i = 1 \ldots N_{res}$

(invariant point attn)

$s_i = \text{Transition}(s_i) + s_i$

$T_i = T_i \circ \underline{\text{BackBoneUpdate}(s_i)}$

$C_s = 384$

N_{res} 1 2 : i : N_{res} $-\vec{s}_i-$

$T_i, \vec{x}_j = \underline{\text{Compute Co-ords}}()$

$$\mathcal{L} = \text{FAPE}\left(\underset{\forall i}{\{T_i\}}, \underset{\forall j}{\{x_j^{c\alpha}\}}, \underset{\forall i}{\{T_i^{true}\}}, \underset{\forall j}{\{x_j^{c\alpha\, true}\}}\right)$$

Frame Aligned Point Error

$i, j = 1 \ldots N_{res}$ for $C\alpha$

$T_i \equiv$ maps from local to global frame per position

$$T_i = (\vec{R}_i, \vec{t}_i)$$

$$T_i(\vec{x}) = \vec{R}_i \cdot \vec{x} + \vec{t}_i \qquad \vec{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

3D coord

$$\underbrace{T_1 \circ \left[T_2 \left(\vec{x}\right)\right]}$$

$T_1 = R_1 \, \vec{t}_1$

$T_2 = R_2 \, \vec{t}_2$

$$T_1\left(R_2 \vec{x} + \vec{t}_2\right)$$

$$R_1 \left(\underbrace{R_2 \vec{x} + \vec{t}_2}\right) + \vec{t}_1$$

$$\underline{R_1 R_2 \vec{x}} + \underline{\underline{R_1 t_2 + \vec{t}_1}}$$

$$R' \vec{x} + t'$$

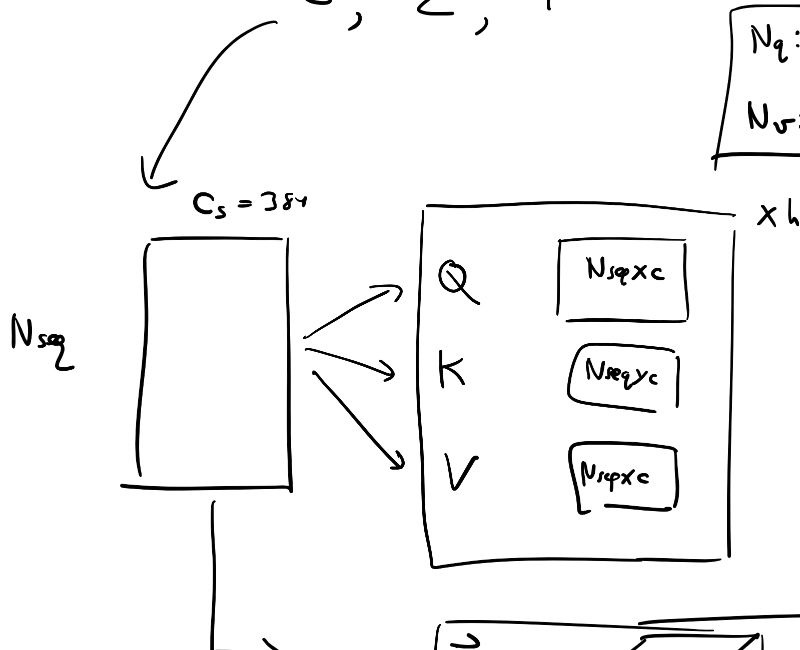
IPA: Invariant Point Attn

$h = 12$

$c = 16$ (d - projection)

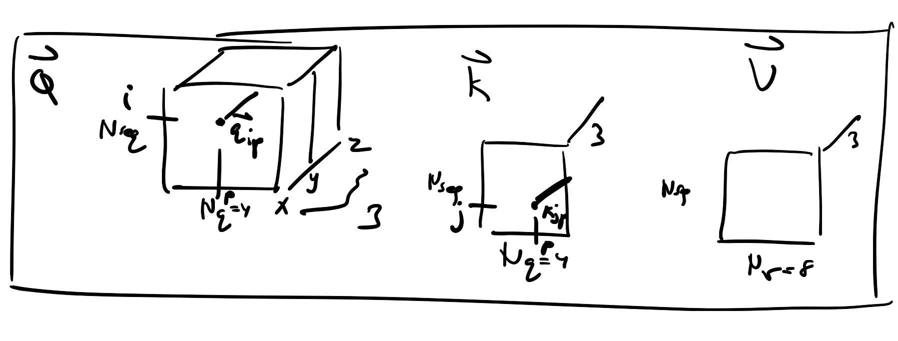
N_q: 4 query points

N_v: 8 value points



3D

$\vec{Q}, \vec{K}, \vec{V}$



$$a_{ij}^h = \underset{=}{w_L}\left(\underbrace{\frac{q_i^{hT} k_j^h}{\sqrt{c}}}_{\text{normal attn}} + b_{ij}^h + \gamma^h \frac{w_c}{2}\sum_p^4 \left\| T_i\left(\vec{q}_{ip}^{\,h}\right) - T_j\left(\vec{k}_{jp}^{\,h}\right)\right\|^2\right)$$

b_{ij}^h: Σ (from pair rep)

γ^h: weight for head h

$$w_L = \frac{1}{\sqrt{3}} \qquad w_c = \sqrt{\frac{2}{9N_q}}$$

Attn: all q_i, k_i, v_i value are sampled IID from $N(0,1)$

IID: Independent & Identially distributed

$N(0,1)$: Normal distribution, $\mu = 0$, $\sigma^2 = 1$

$$\vec{q} \in \mathbb{R}^c \qquad \vec{k} \in \mathbb{R}^c$$

$$\vec{q}^{\,T}\vec{k} = \sum_{i=1}^{c} \underbrace{q_i \cdot k_i}_{\text{Var}(1)}$$

$$= \text{Var}(\underbrace{1+1+1+\cdots+1}_{c \text{ times}}) = c$$

$$\text{Var}\left(\frac{\vec{q}^{\,T}\vec{k}}{\sqrt{c}}\right) = \text{Var}\left(\sum\left(\frac{1}{\sqrt{c}} q_i k_i\right)\right)$$

$$= \text{Var}\left(\frac{1}{\sqrt{c}} + \frac{1}{\sqrt{c}} + \cdots + \frac{1}{\sqrt{c}}\right)$$

squared

$$= \frac{1}{c} + \frac{1}{c} + \cdots + \frac{1}{c}$$

$$= \frac{c}{c} = 1$$

$$\text{Var}(aX + bY) = a^2\,\text{Var}(X) + b^2\,\text{Var}(Y)$$

$$\frac{1}{2}\left(\sum_{p=1}^{N_q}\right) \| \underbrace{T_i(q_{ip})}_{q_i} - \underbrace{T_j(k_{jp})}_{k_j} \|^2$$

$$\underbrace{q_i \quad k_j}_{\in \mathbb{R}^3}$$

$$\| q_i - k_j \|^2 = (q_i - k_j)^T (q_i - k_j)$$

$$= \frac{1}{2}\left(q_i^T q_i - 2 q_i^T k_j + k_j^T k_j\right)$$

$$Var = \left(\left(\frac{q_i^T q_i}{2}\right) - q_i^T k_j + \frac{k_j^T k_j}{2} \right)$$

$$= \frac{1}{4} + \frac{1}{4} + \frac{1}{4} + 1 + 1 + 1 + \frac{1}{4} + \frac{1}{4} + \frac{1}{4}$$

$$= \frac{6}{4} + 3 = \frac{18}{4}$$

Total var $= \frac{N_q \cdot 18}{4}$

divide by $\sqrt{\frac{N_q \cdot 9}{2}}$

$$W_c = \frac{1}{\sqrt{\frac{9 N_q}{2}}} = \sqrt{\frac{2}{9 N_q}}$$

$$a_{ij} = \left(\underline{\text{Normal} + \text{bias} + \sum \underline{\text{3d attn}}} \right) \leftarrow$$

$$\tilde{o}_i = \sum_j a_{ij} z_{ij} \nwarrow \sum$$

$$o_i = \sum_j a_{ij} v_j \leftarrow \text{Normal value}$$

$$o_i^p = T_i^{-1}\left(\underbrace{\sum_j a_{ij}\left(T_j(\vec{v}_j)\right)}_{\text{global ref frame}}\right)$$

$$\underline{\qquad\qquad\qquad\qquad}$$

local ref frame

$$s_i = \text{linear}\left(\text{concat}\left(\tilde{o}_i, o_i, \underbrace{o_i^p, \|o_i^p\|}_{N_v = 8 \text{ of these}}\right)\right)$$

$\downarrow$

$384 = c_s$