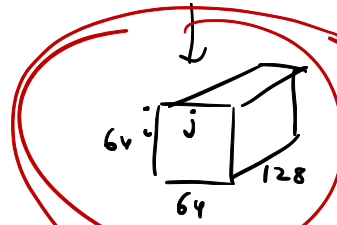
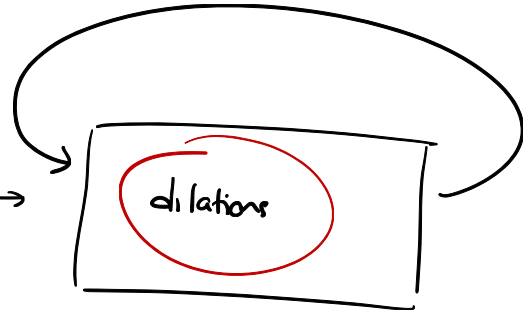
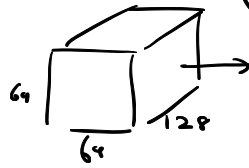
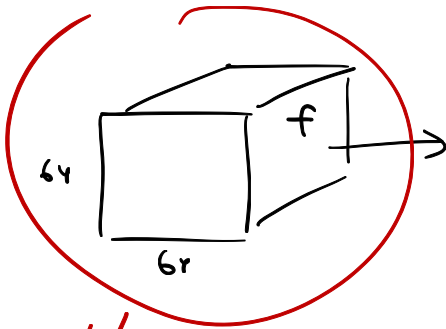


Angle prediction

↳ optional for Assignment

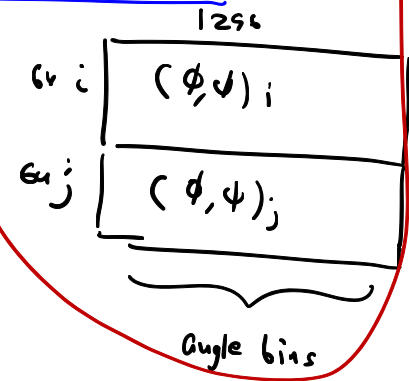
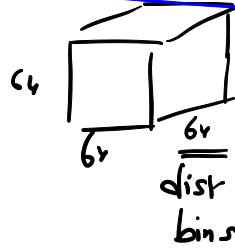


Distance

Angle

final $\mathcal{L} =$

$$\text{CE-loss} + \text{CE-loss}$$



vs

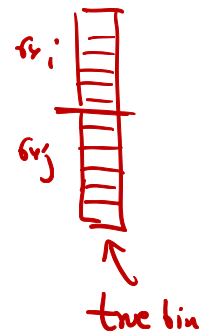
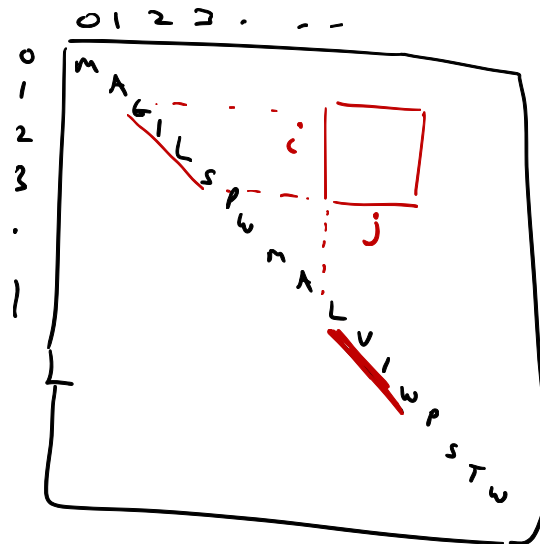
Pytorch

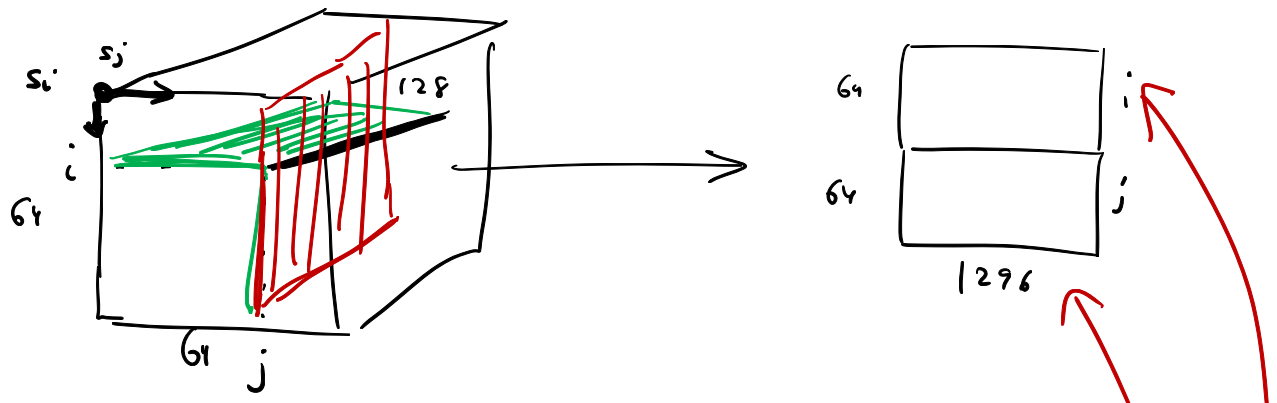
C: channels come first

~~64 x 64 x f~~
f x 64 x 64

0 1 2 3 . . .
M A G I L S P W W M A L V I W P S T W
i j

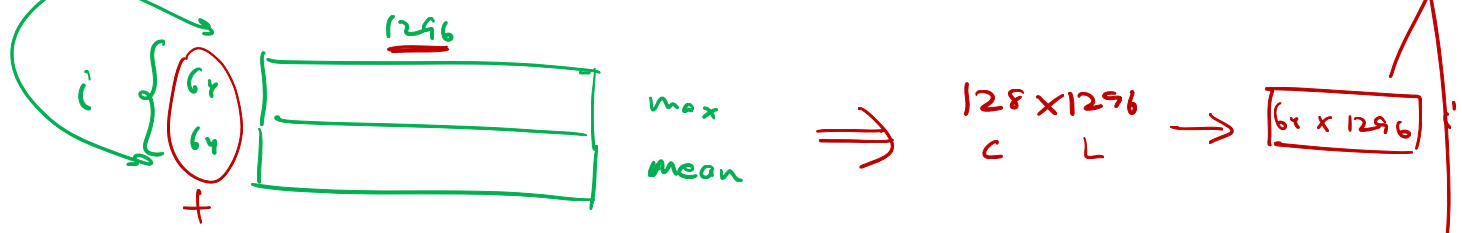
Crop size 4





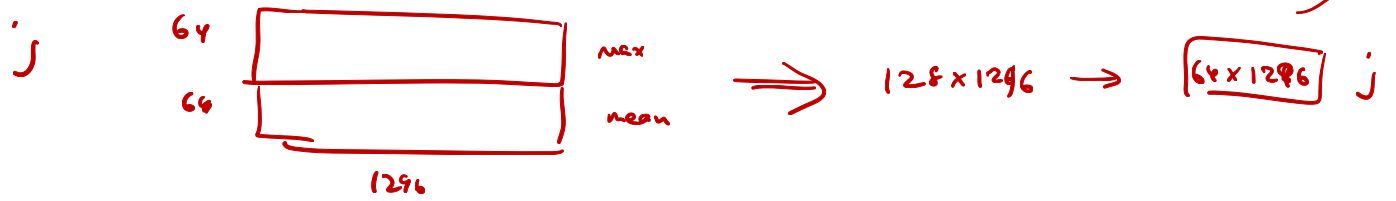
Max 2d pool ($\frac{128}{in}$, $\frac{1296}{out}$, $\frac{1 \times 64}{kernel}$, ...)

Mean 2d pool ()

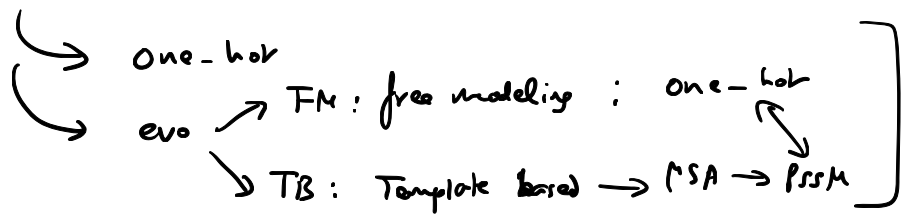
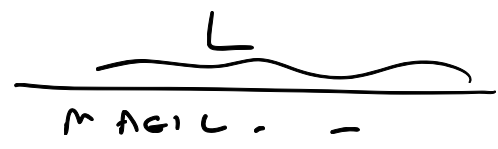


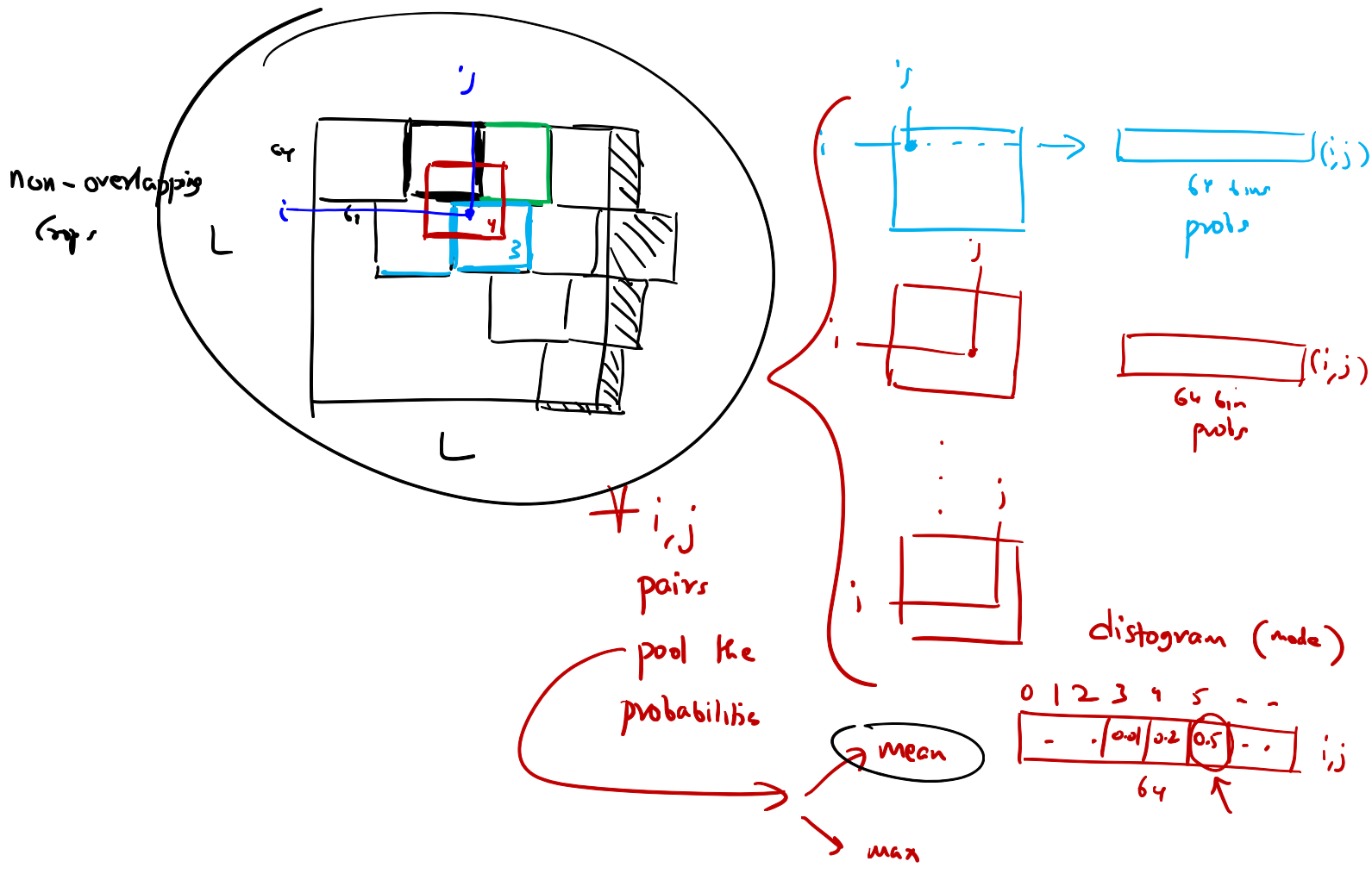
max 2d pool (128, 1296, $\frac{64 \times 1}{kernel}$, ...)

mean 2d pool (128, 1296, $\frac{64 \times 1}{kernel}$, ...)

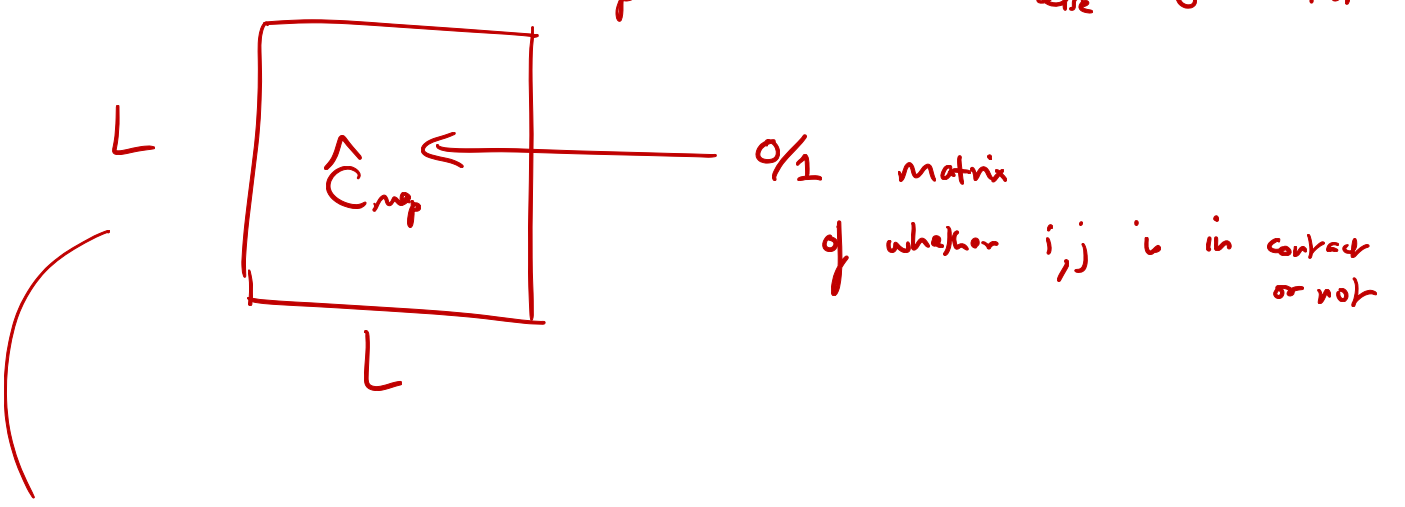
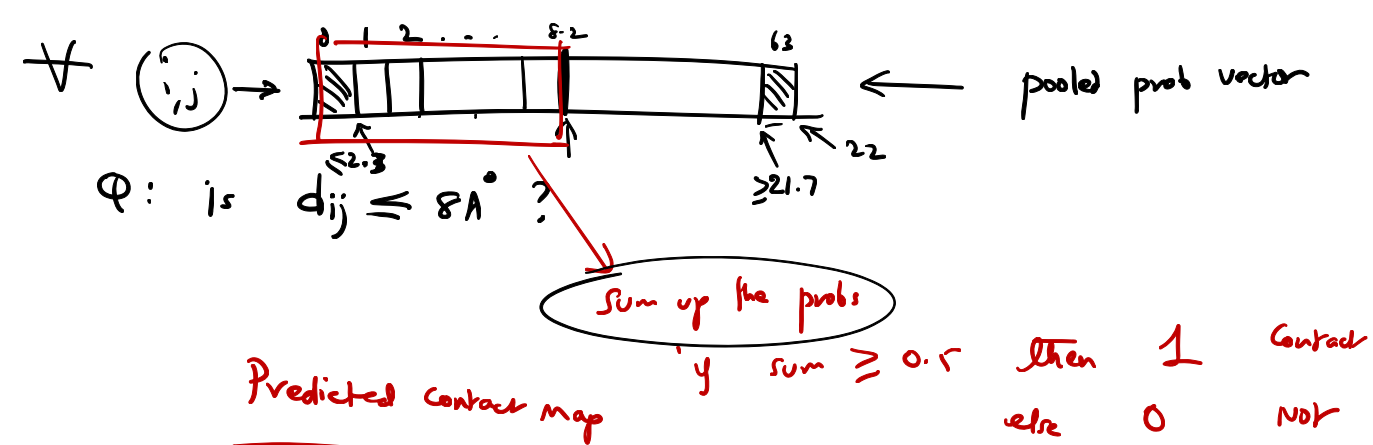


Testing

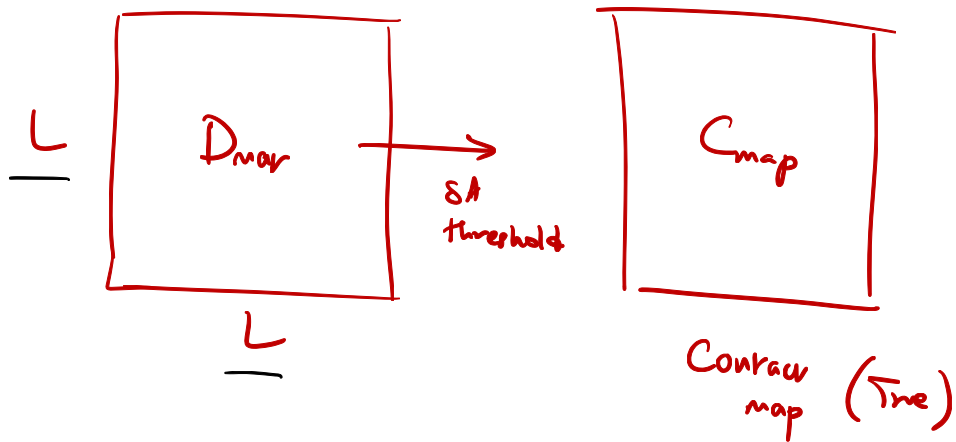




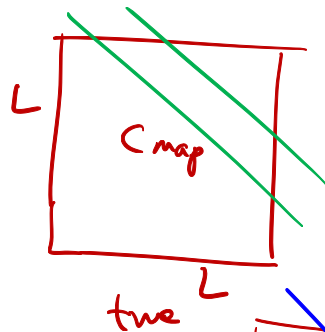
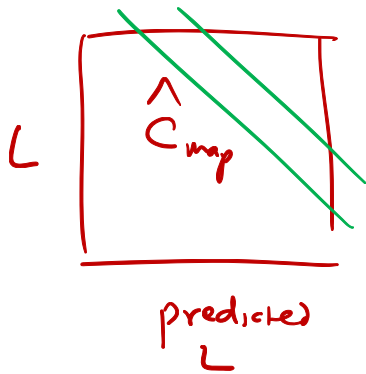
Contact prediction



vs. ground truth contact map



Global Contact Accuracy



Metric: (recall)

$$\frac{\# \text{ of correct}}{\# \text{ of contacts (in true)}}$$

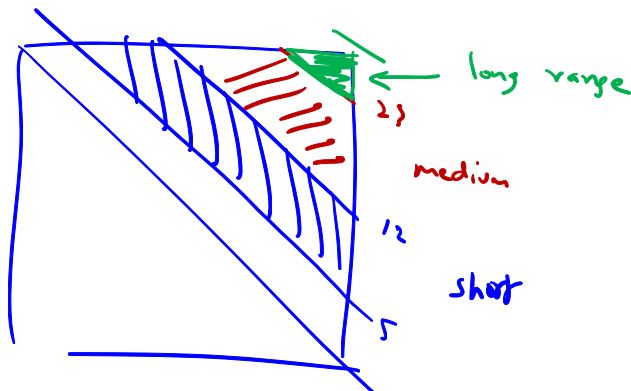
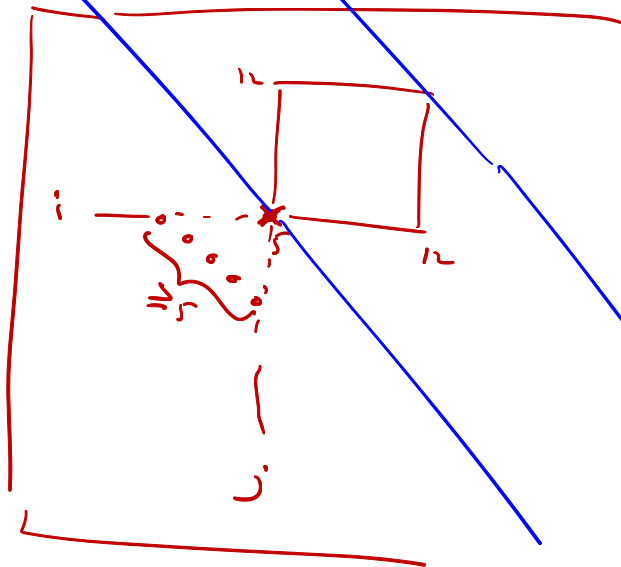
distance based

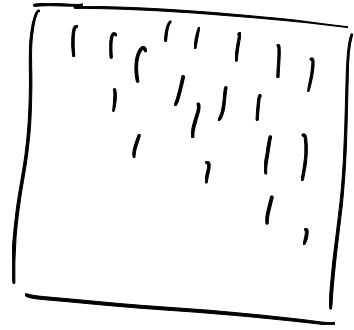
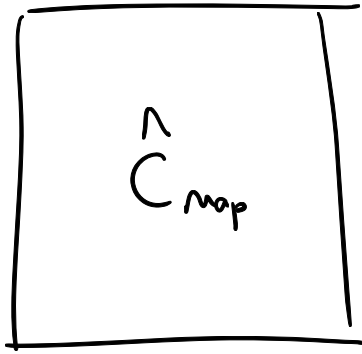
$$5 \leq |i-j| \leq 12$$

seq separation

$$12 < |i-j| \leq 23 \quad \text{medium}$$

$$23 < |i-j| : \text{long}$$

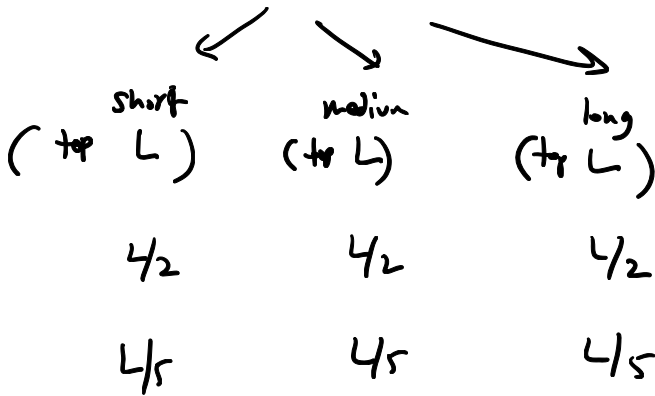




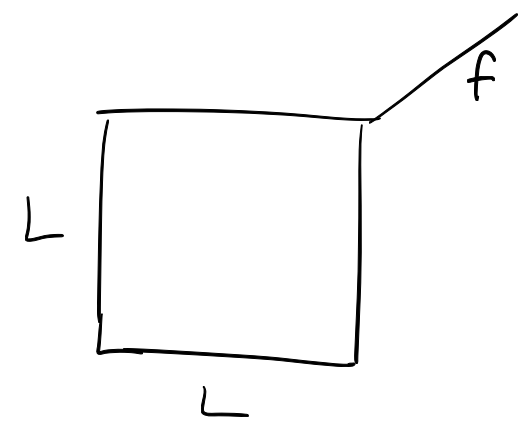
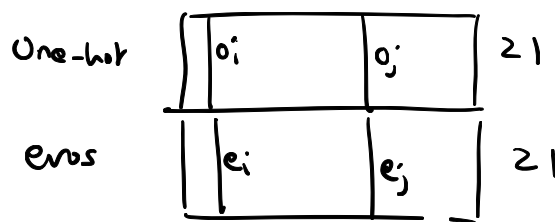
Choose the top L predictions only!
 (i, j) pairs

(sort in decreasing order of the
 sum of the bin probs
 from 0 ... upto the bin
 with δA^*)

Global: out of these L how many are correct!



L



$T: L \times L \times f$

for $\underline{i} = 0 \dots L-1$

for $\underline{j} = 0 \dots L-1$

$$T[i, j] = \underbrace{0_i \parallel 0_j \parallel e_i \parallel e_j \parallel |e_i - e_j|}_{f_{ij}} \parallel e_i \otimes e_j$$

