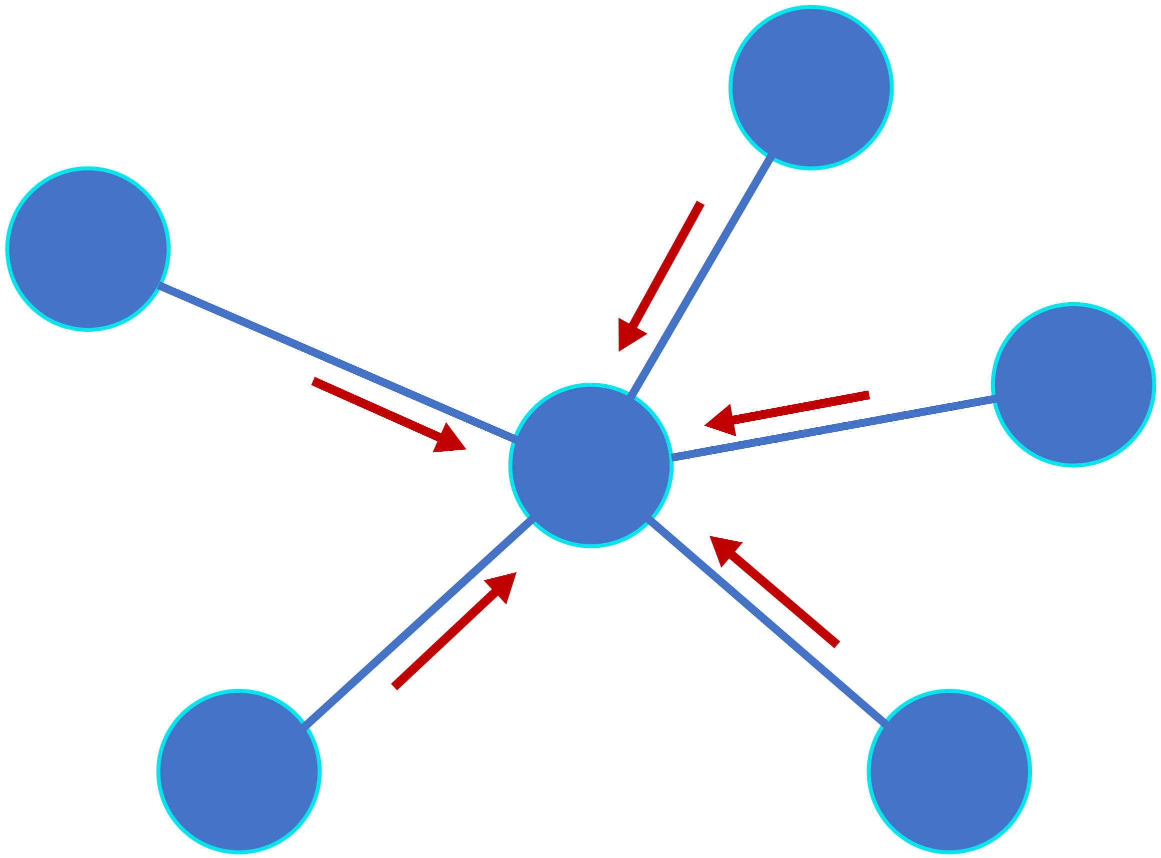
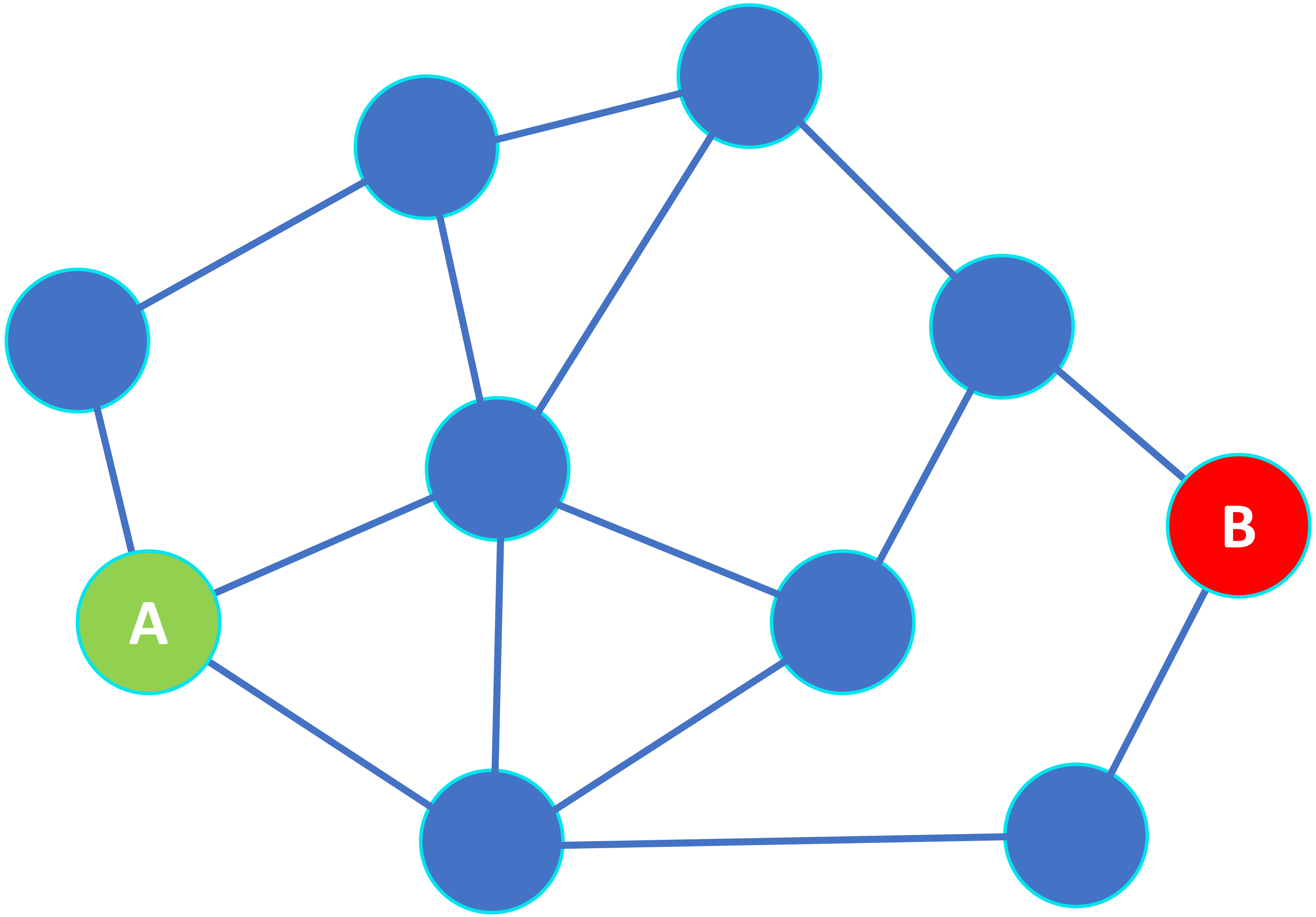
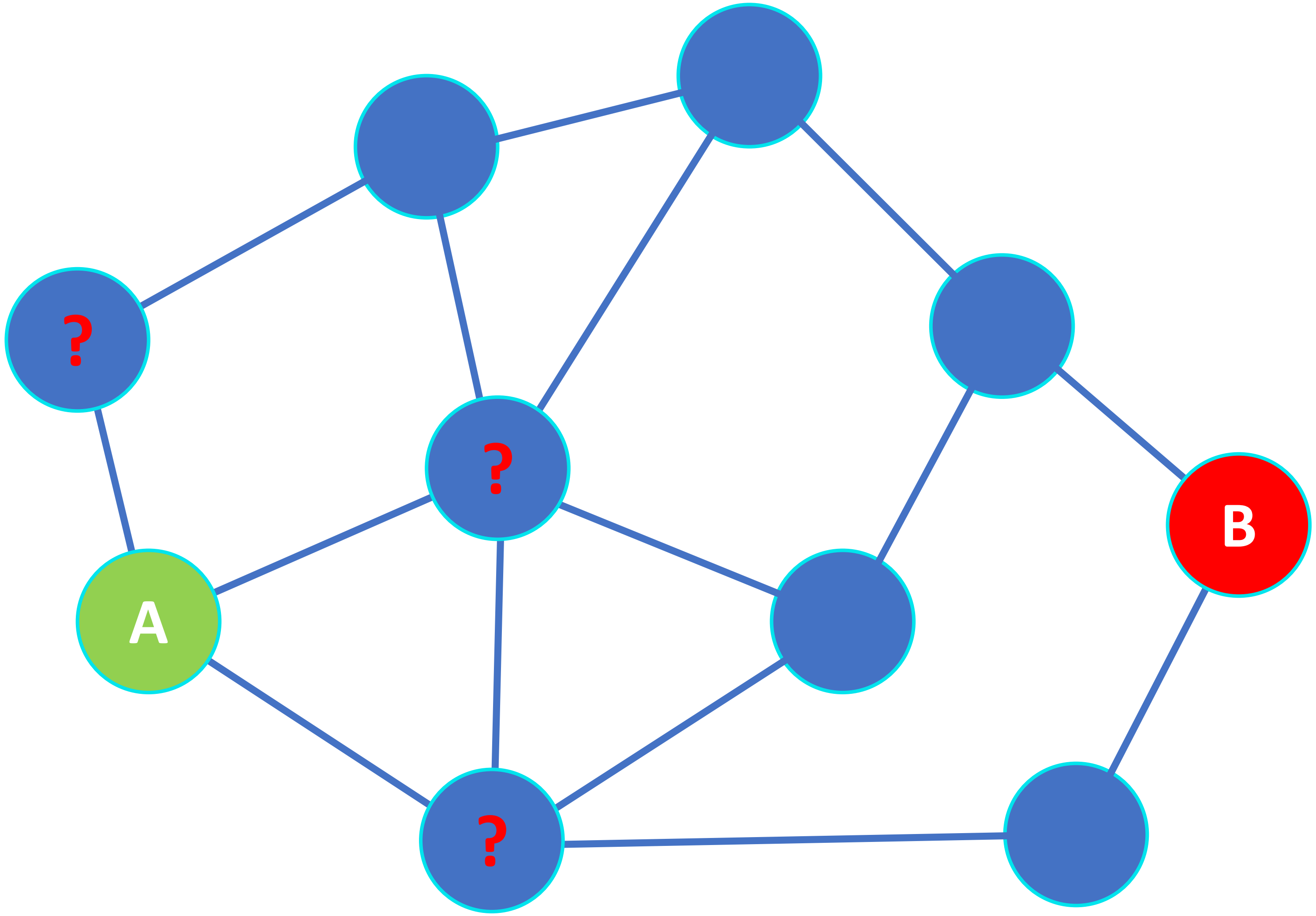
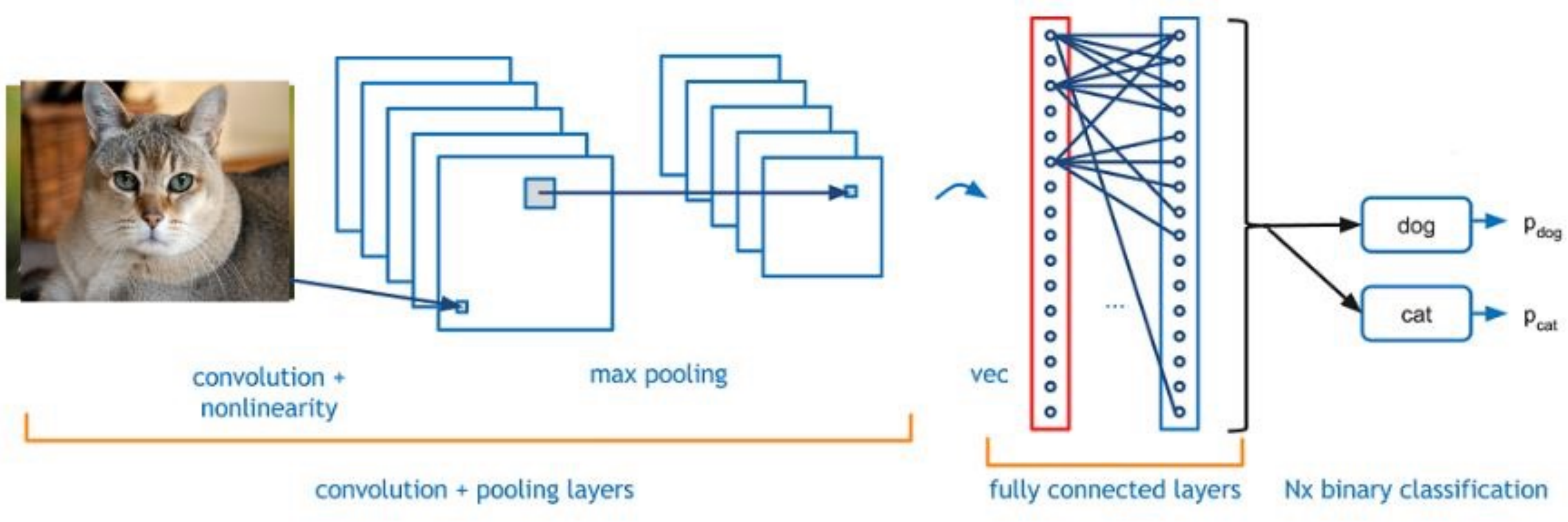
Graph U-Nets

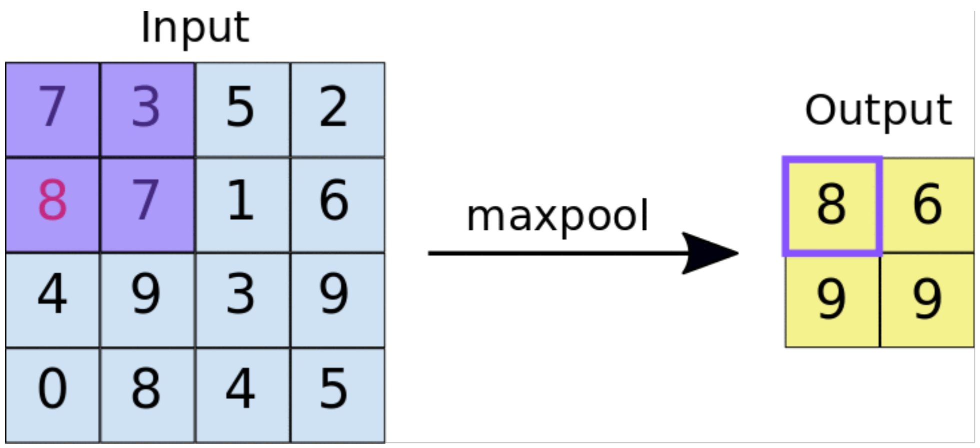
Hongyang Gao Shuiwang Ji

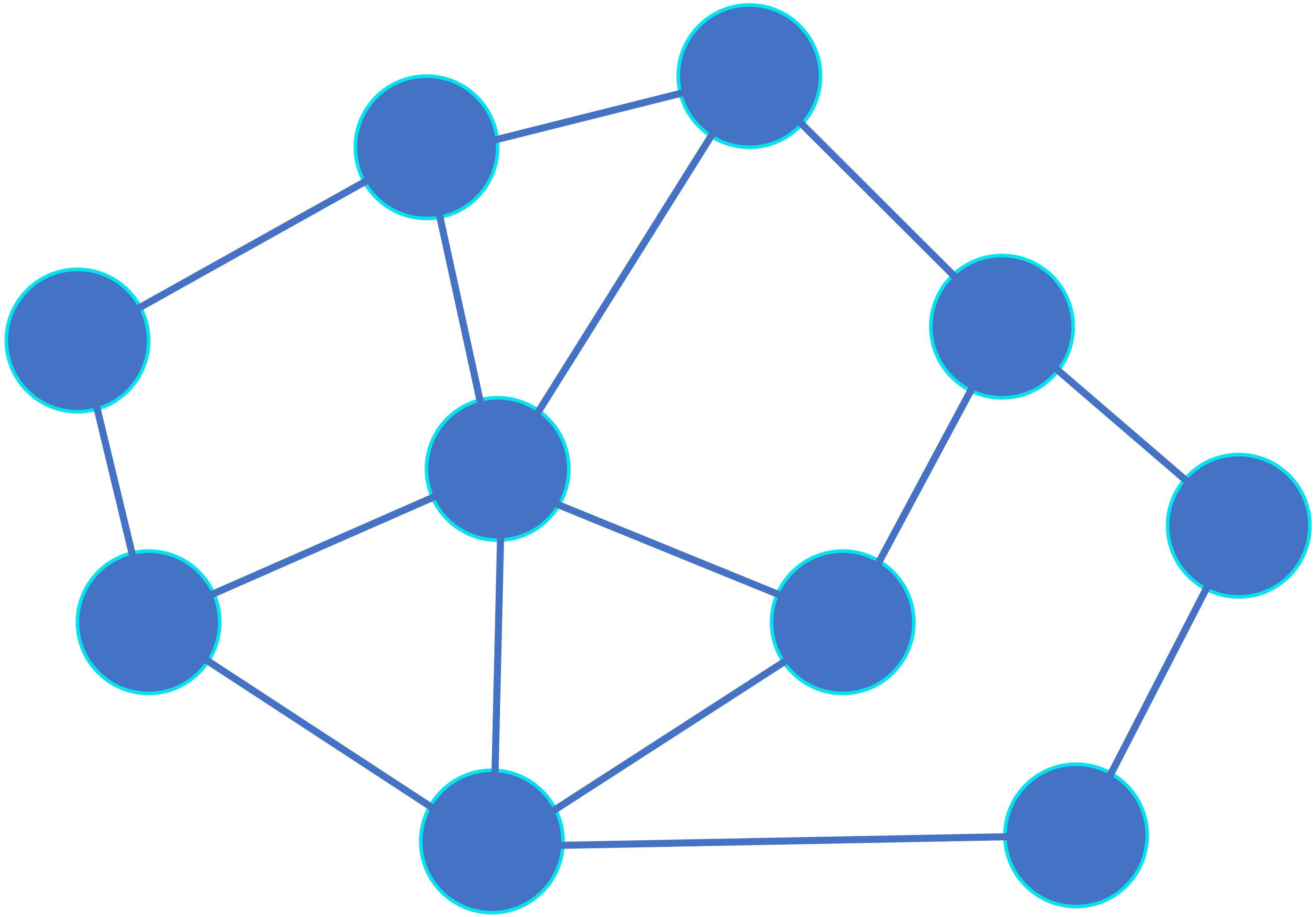


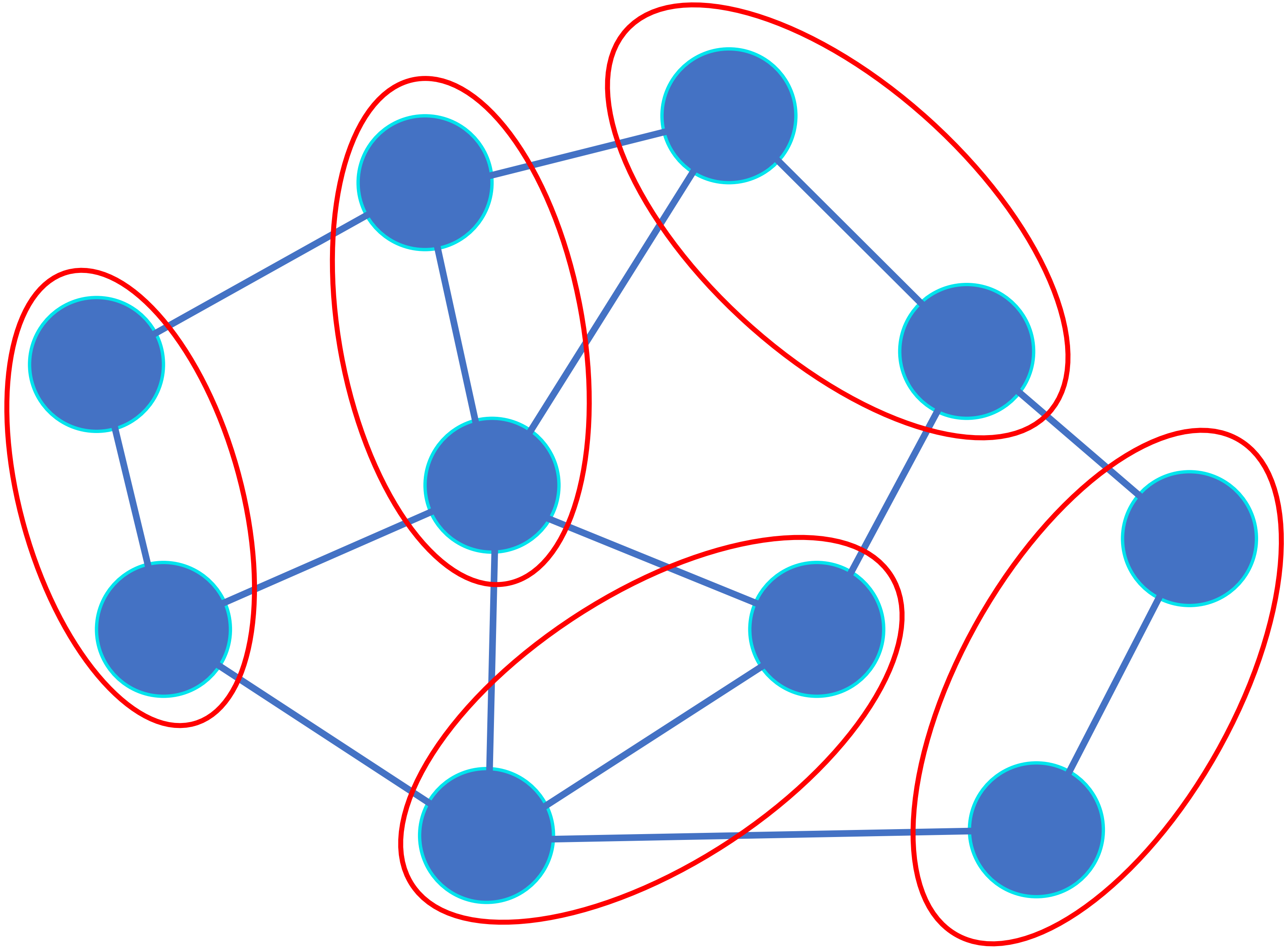

A
B

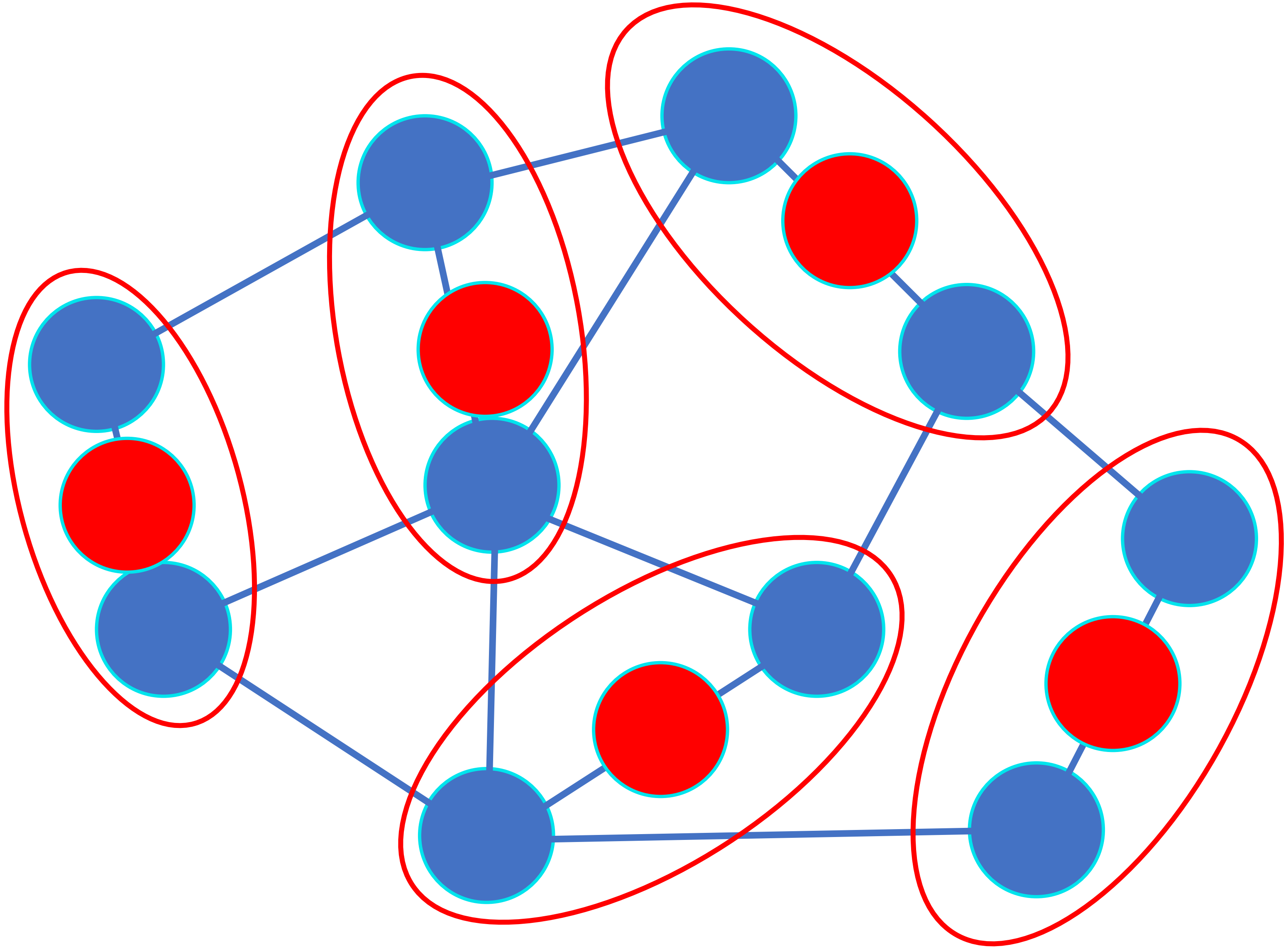

?
?
A
B
?

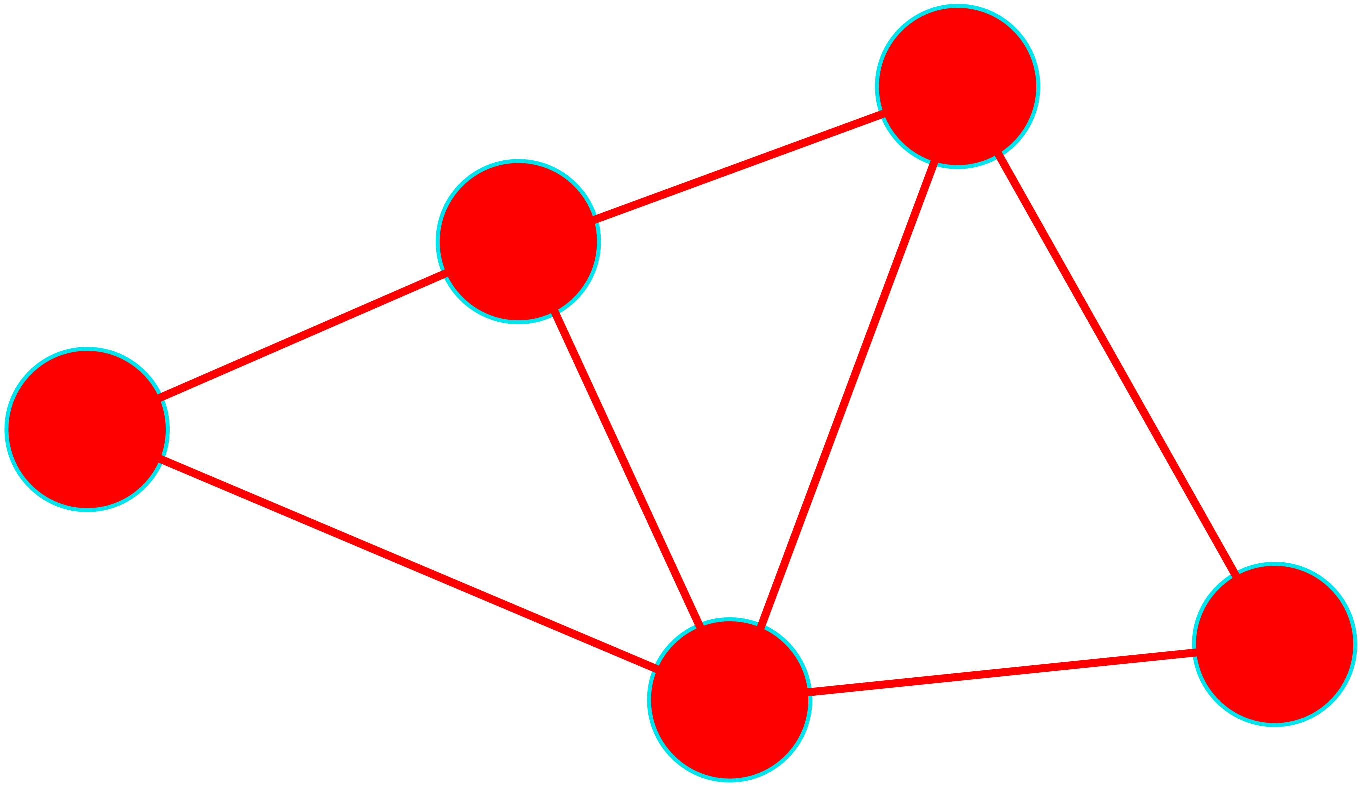

convolution +
nonlinearity
max pooling
vec
dog
cat
p_{dog}
p_{cat}
convolution + pooling layers
fully connected layers
Nx binary classification


Input
7 3 5 2
8 7 1 6
4 9 3 9
0 8 4 5
maxpool
Output
8 6
9 9









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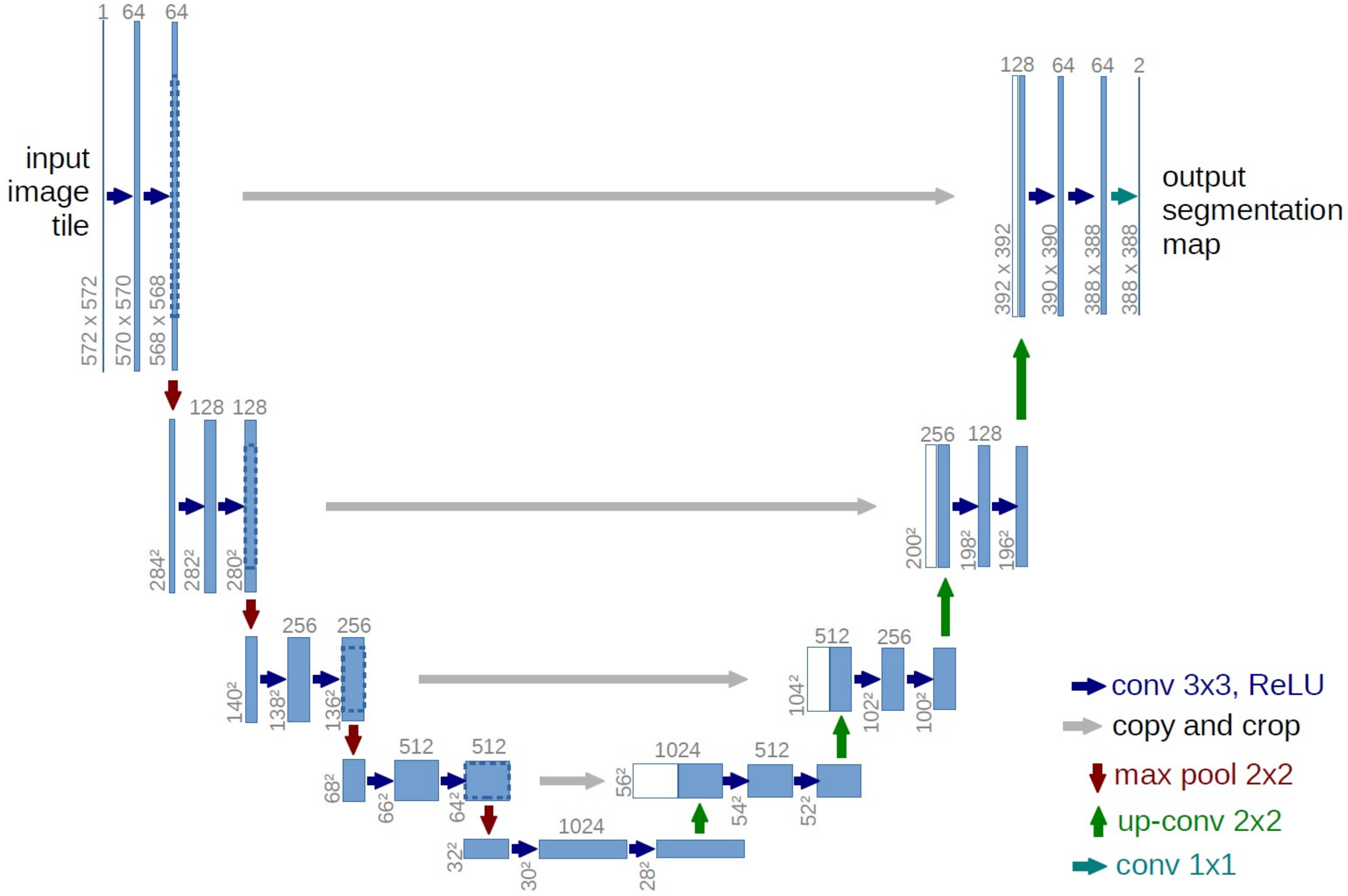
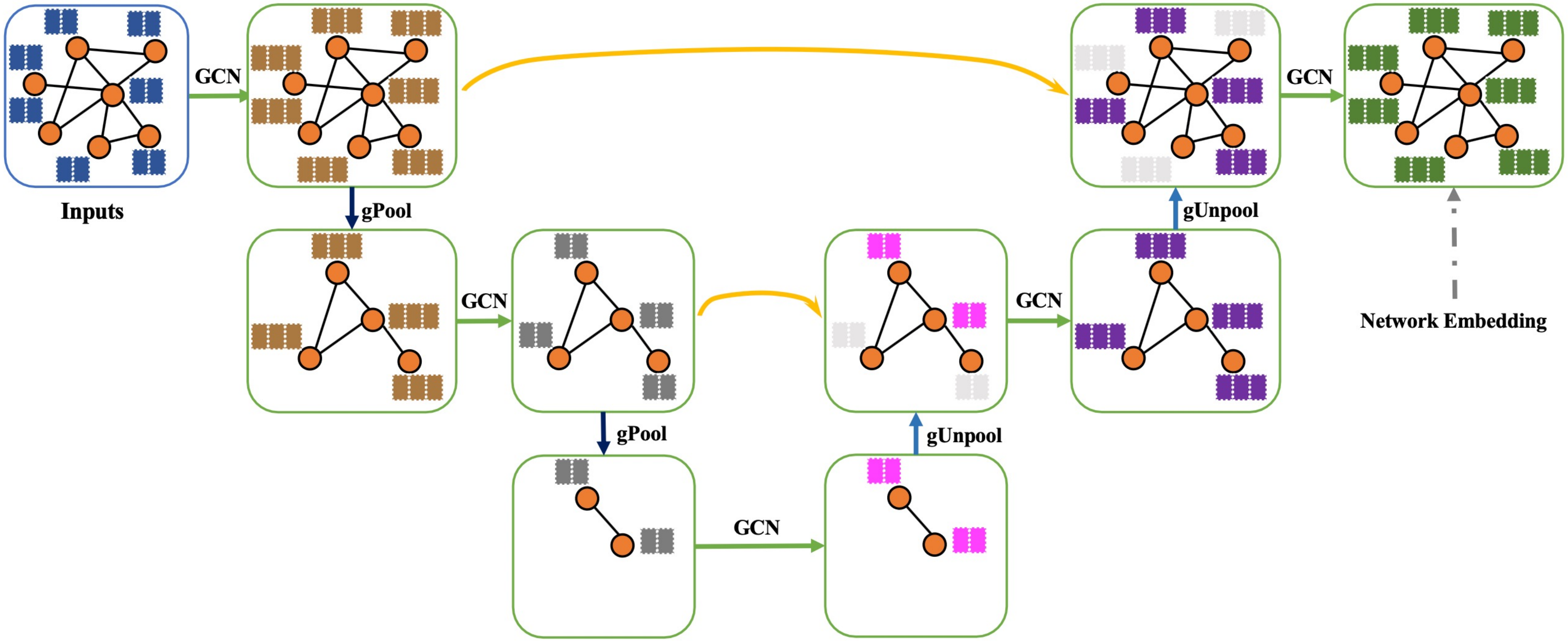
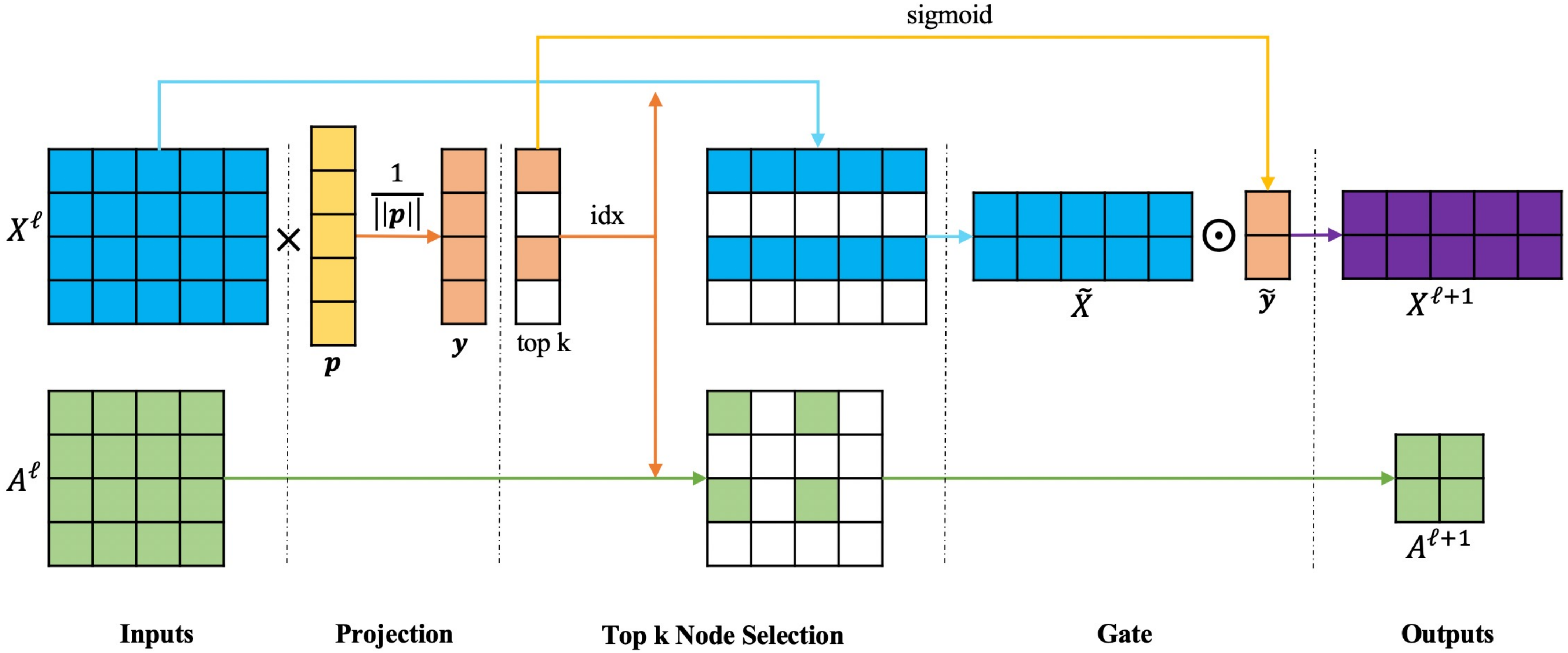
U-Net :



input image tile
output segmentation map
1
64
64
572 x 572
570 x 570
568 x 568
128
128
284²
282²
280²
256
256
140²
138²
136²
512
512
68²
66²
64²
1024
32²
30²
28²
1024
512
56²
54²
52²
512
256
104²
102²
100²
256
128
200²
198²
196²
128
64
64
2
392 x 392
390 x 390
388 x 388
388 x 388
conv 3x3, ReLU
copy and crop
max pool 2x2
up-conv 2x2
conv 1x1

Graph U-Net :


GCN
Inputs
gPool
GCN
gPool
GCN
gUnpool
GCN
gUnpool
GCN
Network Embedding



$$
\begin{aligned}
\mathbf{y} &= X^\ell \mathbf{p}^\ell / \|\mathbf{p}^\ell\|, \\
\mathrm{idx} &= \mathrm{rank}(\mathbf{y}, k), \\
\tilde{\mathbf{y}} &= \mathrm{sigmoid}(\mathbf{y}(\mathrm{idx})), \\
\tilde{X}^\ell &= X^\ell(\mathrm{idx}, :), \\
A^{\ell+1} &= A^\ell(\mathrm{idx}, \mathrm{idx}), \\
X^{\ell+1} &= \tilde{X}^\ell \odot \left(\tilde{\mathbf{y}} \mathbf{1}_C^T\right),
\end{aligned}
$$

Table 3. Results of transductive learning experiments in terms of node classification accuracies on Cora, Citeseer, and Pubmed datasets. g-U-Nets denotes our proposed graph U-Nets model.

Models	**Cora**	**Citeseer**	**Pubmed**
DeepWalk (Perozzi et al., 2014)	67.2%	43.2%	65.3%
Planetoid (Yang et al., 2016)	75.7%	64.7%	77.2%
Chebyshev (Defferrard et al., 2016)	81.2%	69.8%	74.4%
GCN (Kipf & Welling, 2017)	81.5%	70.3%	79.0%
GAT (Veličković et al., 2017)	$83.0 \pm 0.7\%$	$72.5 \pm 0.7\%$	$79.0 \pm 0.3\%$
g-U-Nets (Ours)	$\mathbf{84.4 \pm 0.6\%}$	$\mathbf{73.2 \pm 0.5\%}$	$\mathbf{79.6 \pm 0.2\%}$

Table 4. Results of inductive learning experiments in terms of graph classification accuracies on D&D, PROTEINS, and COLLAB datasets. g-U-Nets denotes our proposed graph U-Nets model.

Models	**D&D**	**PROTEINS**	**COLLAB**
PSCN (Niepert et al., 2016)	76.27%	75.00%	72.60%
DGCNN (Zhang et al., 2018)	79.37%	76.26%	73.76%
DiffPool-DET (Ying et al., 2018)	75.47%	75.62%	**82.13%**
DiffPool-NOLP (Ying et al., 2018)	79.98%	76.22%	75.58%
DiffPool (Ying et al., 2018)	80.64%	76.25%	75.48%
g-U-Nets (Ours)	**82.43%**	**77.68%**	77.56%