

Capsule Graph Neural Network

Zhang et al., ICLR 2019

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Jae-Won Chung

Seoul National University

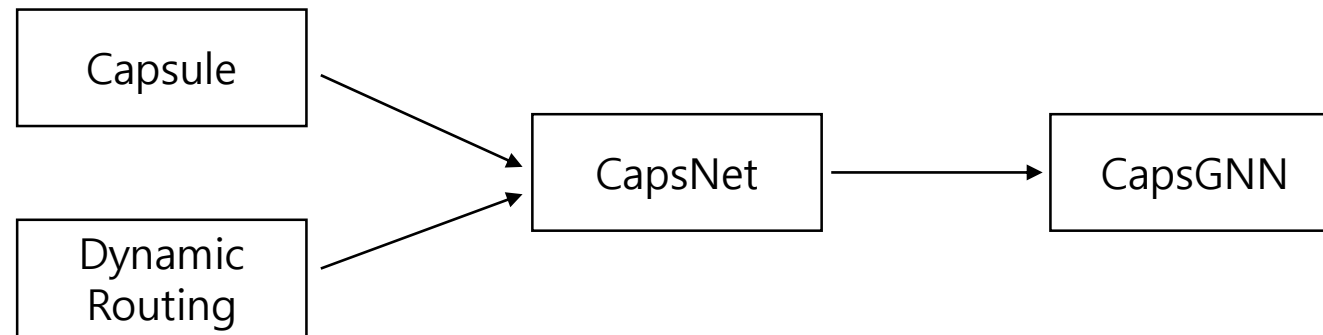


The Idea of Capsules

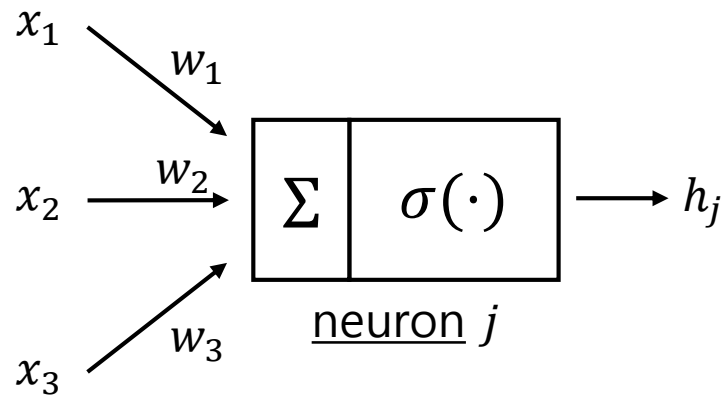
[Transforming Auto-encoders](#), Hinton et al., 2011

[Dynamic Routing between Capsules](#), Sabour et al., 2017

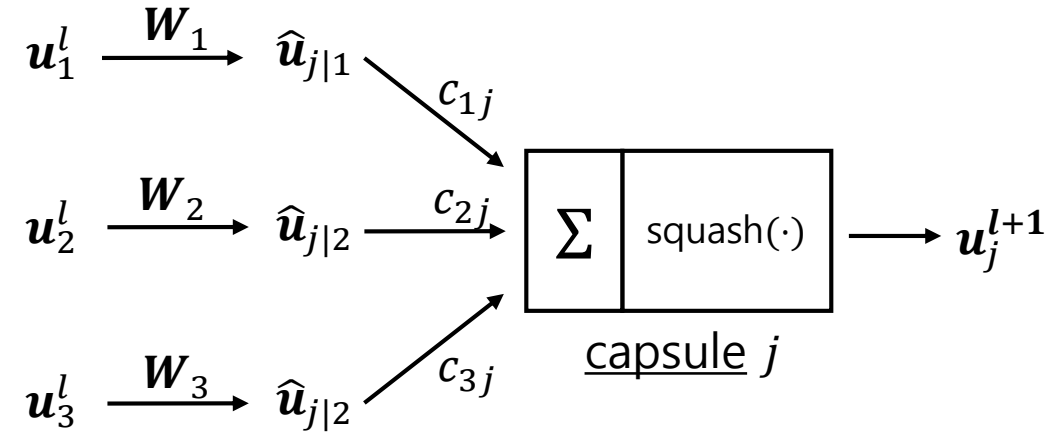
[Capsule Graph Neural Network](#), Zhang et al., 2019



CapsNet: Components



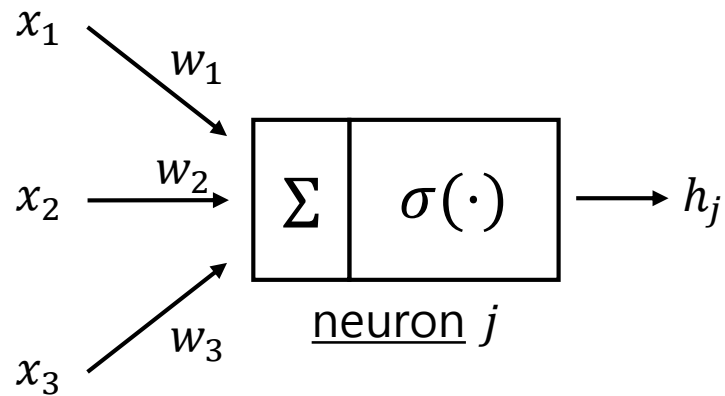
- scalar in scalar out
 - intensity of filter match
- max pool on h_j loses information



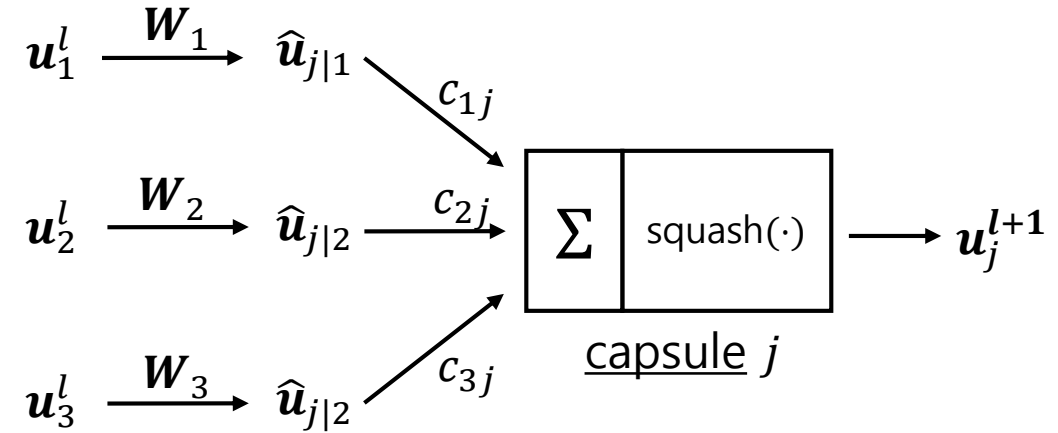
- vector in vector out
 - length: the probability of existence
 - orientation: the entity's current state
- no max pool; preserves information



CapsNet: Components



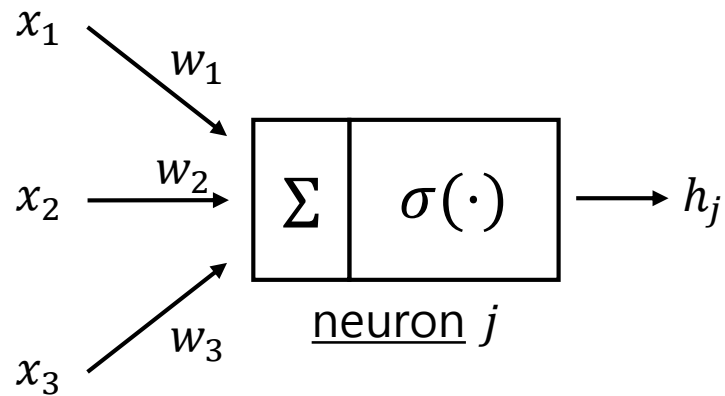
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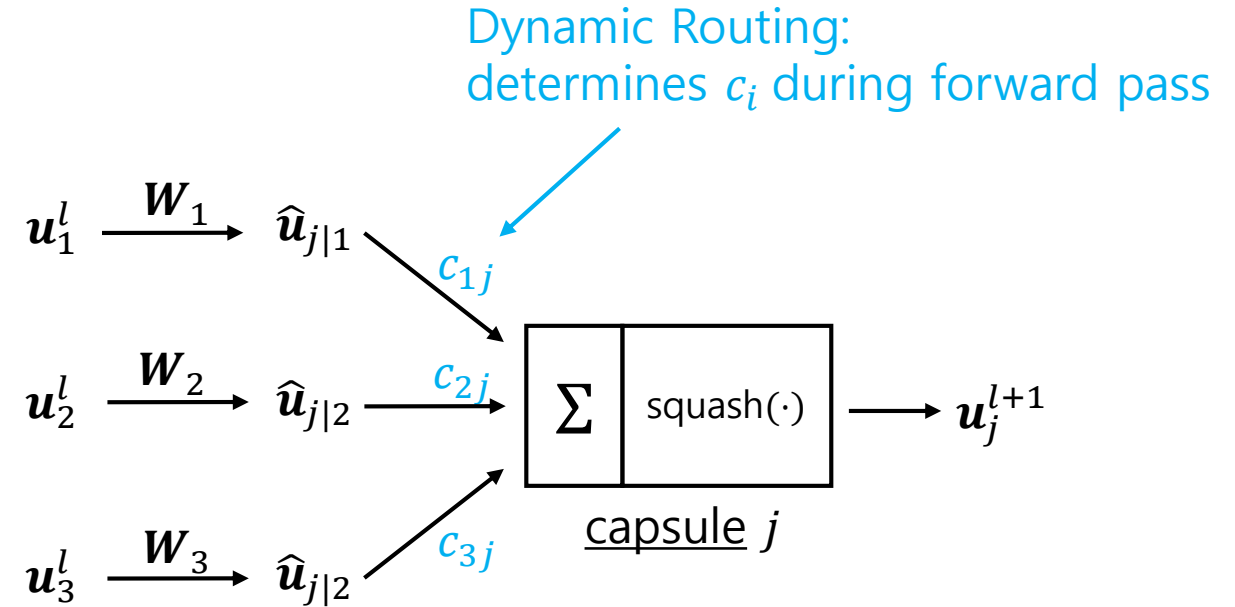
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CapsNet: Components



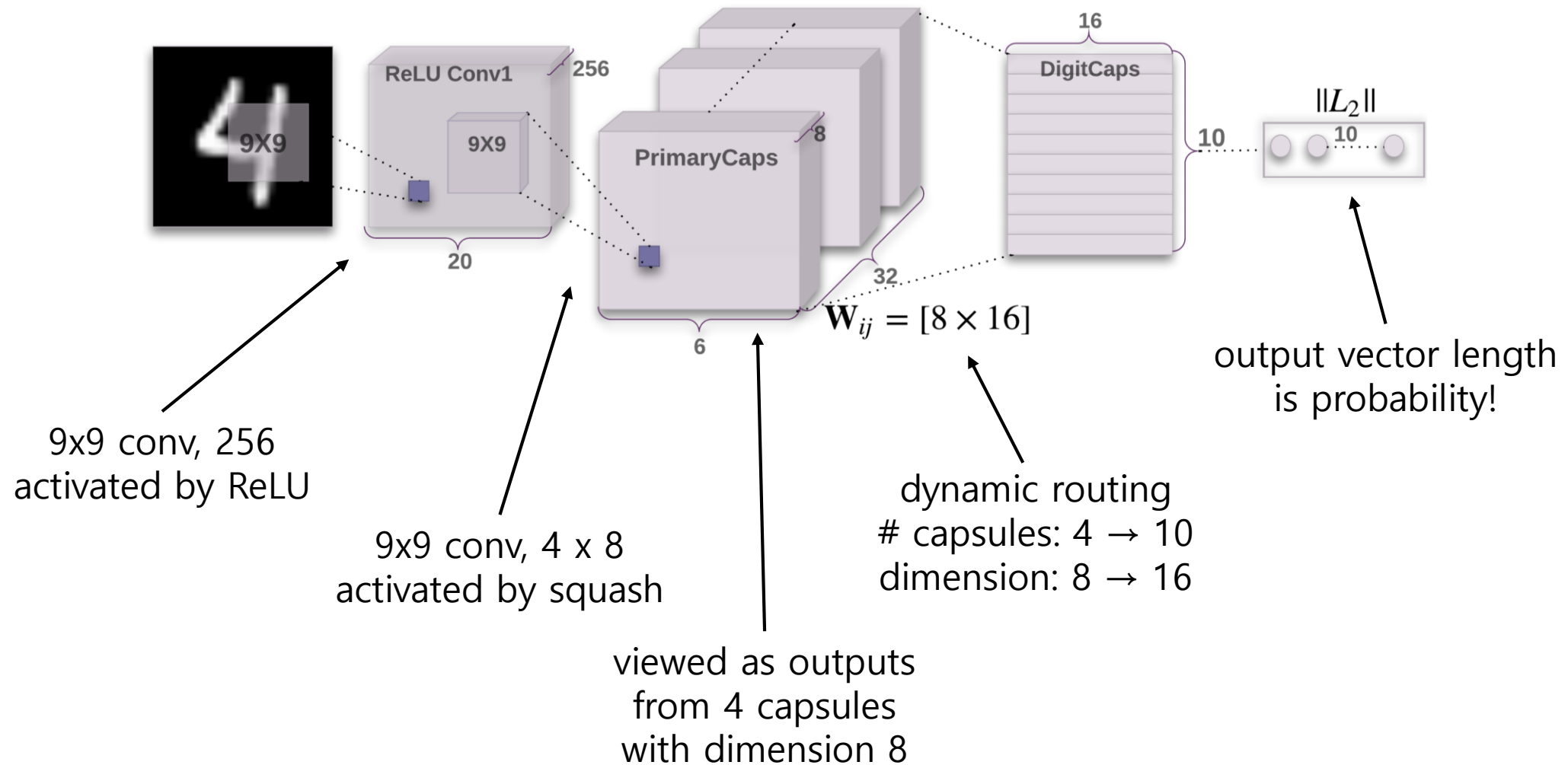
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CapsNet: Architecture

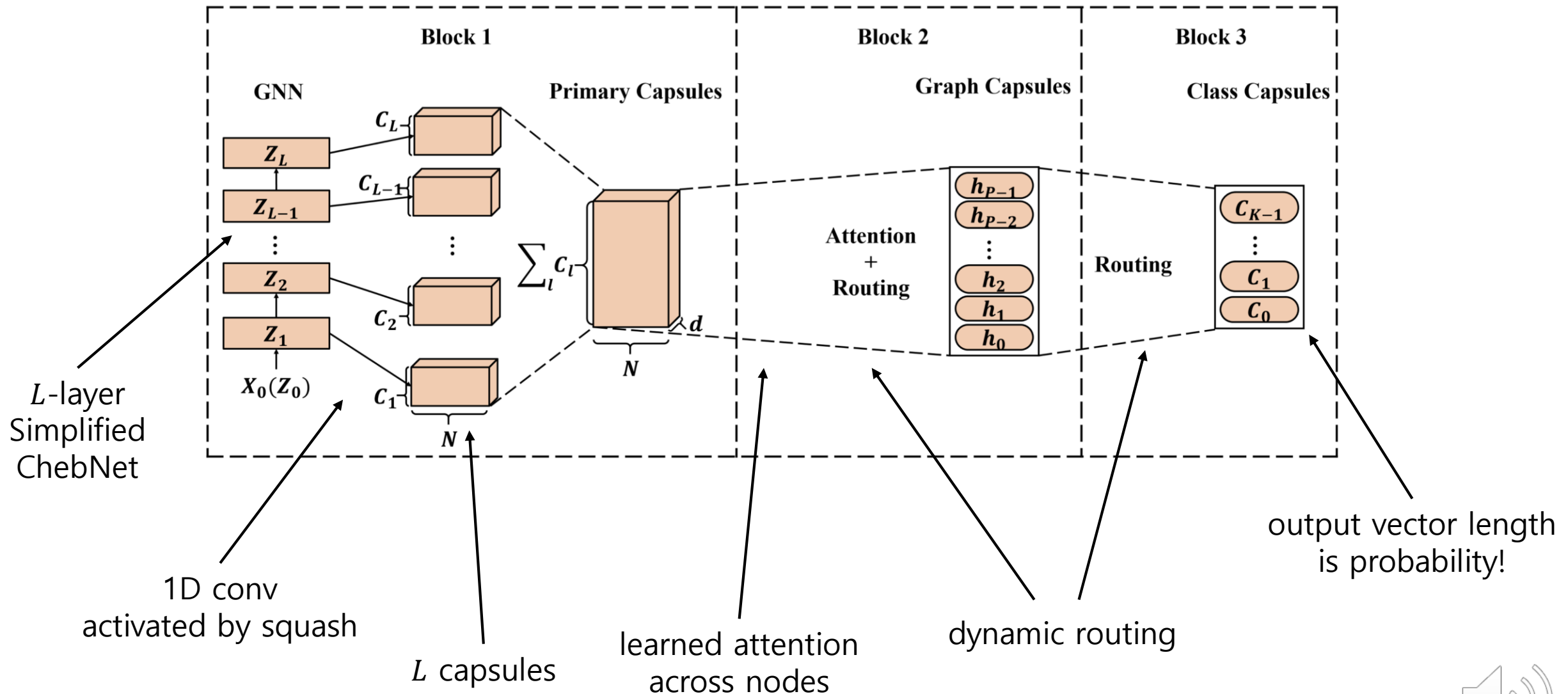


CapsGNN: Motivation

- Simple aggregations in GCNs treat the learned node embeddings as merely an array of scalar features, rather than a meaningful vector in the feature space.
 - Element-wise max-pooling on the node features [Zhang et al., 2018]
 - Taking the element-wise covariance across nodes [Verma & Zhang, 2018]
- Graph embeddings must also capture the position of and structure around each node. Scalar neuron outputs lack representation power.



CapsGNN: Architecture



CapsGNN: Evaluation

biological datasets

Algorithm	MUTAG	NCI1	PROTEINS	D&D	ENZYMES
WL	82.05±0.36	82.19±0.18	74.68±0.49	79.78±0.36	52.22±1.26
GK	81.58±2.11	62.49±0.27	71.67±0.55	78.45±0.26	32.70±1.20
RW	79.17±2.07	>3days	74.22±0.42	>3days	24.16±1.64
Graph2vec	83.15±9.25	73.22±1.81	73.30±2.05	-	-
AWE	87.87±9.76	-	-	71.51±4.02	35.77±5.93
DGK	87.44±2.72	80.31±0.46	75.68±0.54	73.50±1.01	53.43±0.91
PSCN	88.95±4.37	76.34±1.68	75.00±2.51	76.27±2.64	-
DGCNN	85.83±1.66	74.44±0.47	75.54±0.94	79.37±0.94	51.00±7.29
ECC	76.11	76.82	-	72.54	45.67
GCAPS-CNN	-	82.72±2.38	76.40±4.17	77.62±4.99	61.83±5.39
CapsGNN	86.67±6.88	78.35±1.55	76.28±3.63	75.38±4.17	54.67±5.67

social datasets

Algorithm	COLLAB	IMDB-B	IMDB-M	RE-M5K	RE-M12K
WL	79.02±1.77	73.40±4.63	49.33±4.75	49.44±2.36	38.18±1.30
GK	72.84±0.28	65.87±0.98	43.89±0.38	41.01±0.17	31.82±0.08
DGK	73.09±0.25	66.96±0.56	44.55±0.52	41.27±0.18	32.22±0.10
AWE	73.93±1.94	74.45±5.83	51.54±3.61	50.46±1.91	39.20±2.09
PSCN	72.60±2.15	71.00±2.29	45.23±2.84	49.10±0.70	41.32±0.42
DGCNN	73.76±0.49	70.03±0.86	47.83±0.85	48.70±4.54	-
GCAPS-CNN	77.71±2.51	71.69±3.40	48.50±4.10	50.10±1.72	-
CapsGNN	79.62±0.91	73.10±4.83	50.27±2.65	52.88±1.48	46.62±1.90

approaches or surpasses SOTA on 6 of 10 datasets

