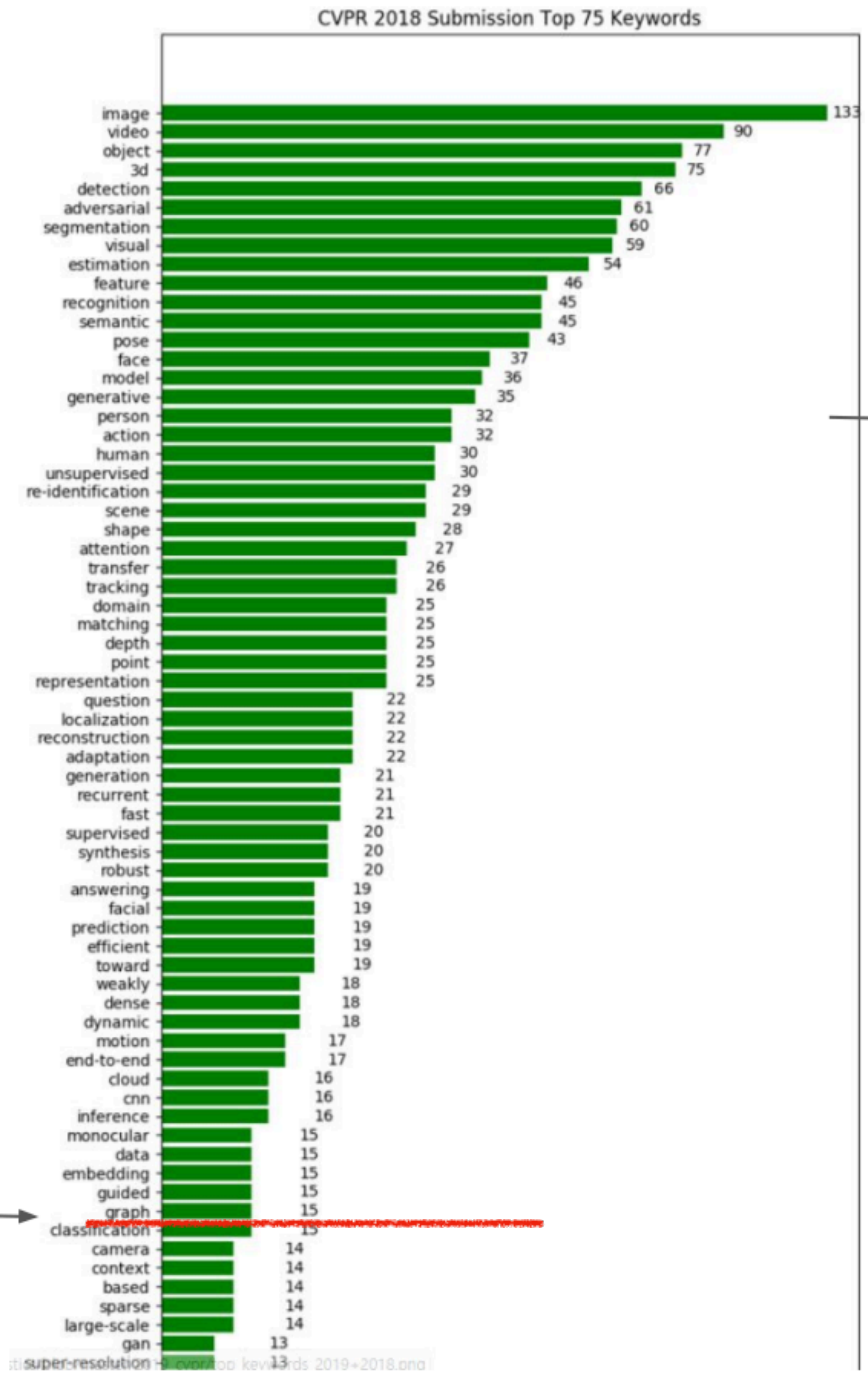
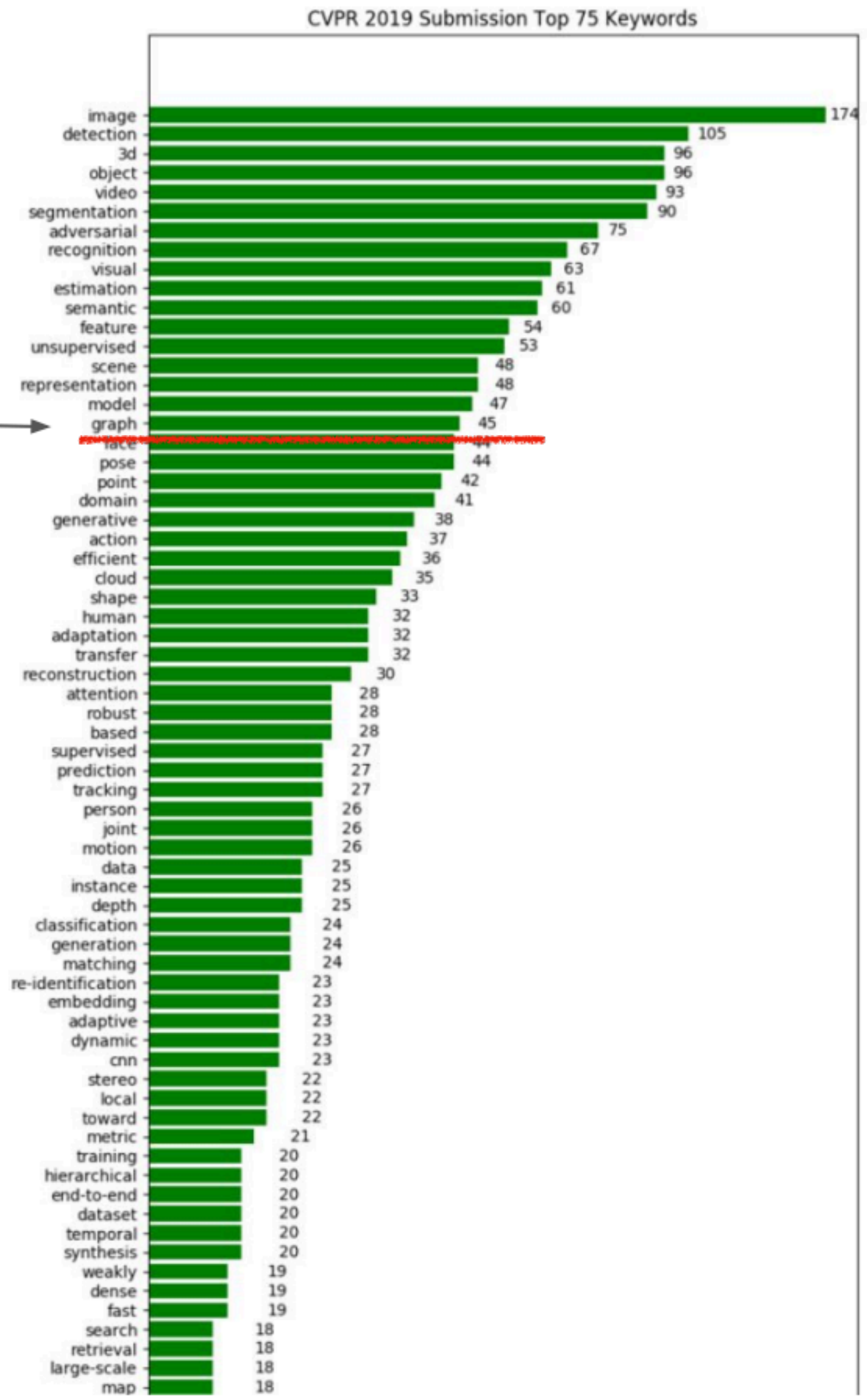
Graph Convolutional Network

Jaeyoung Cheong

1. Trend

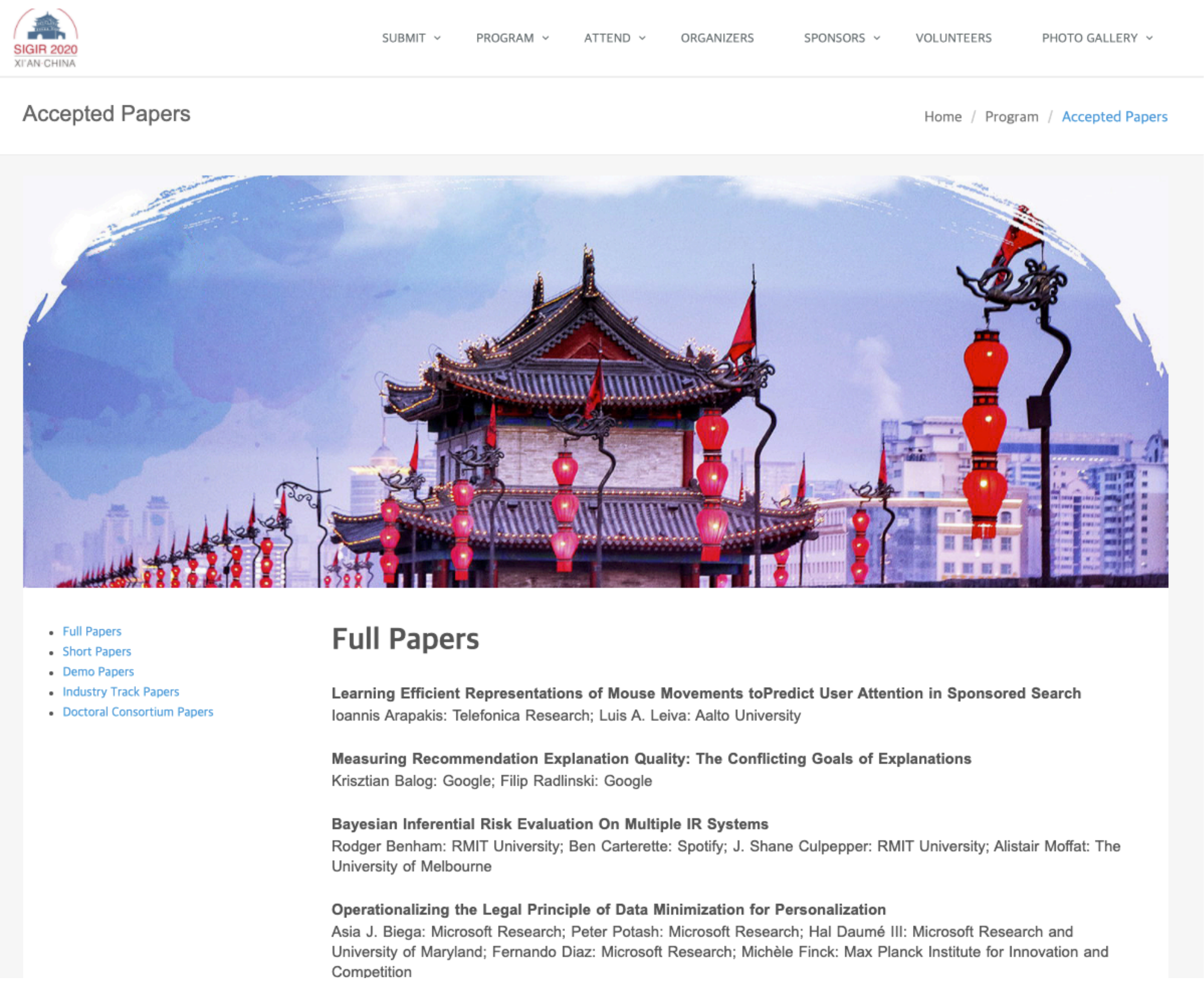
2019 CVPR





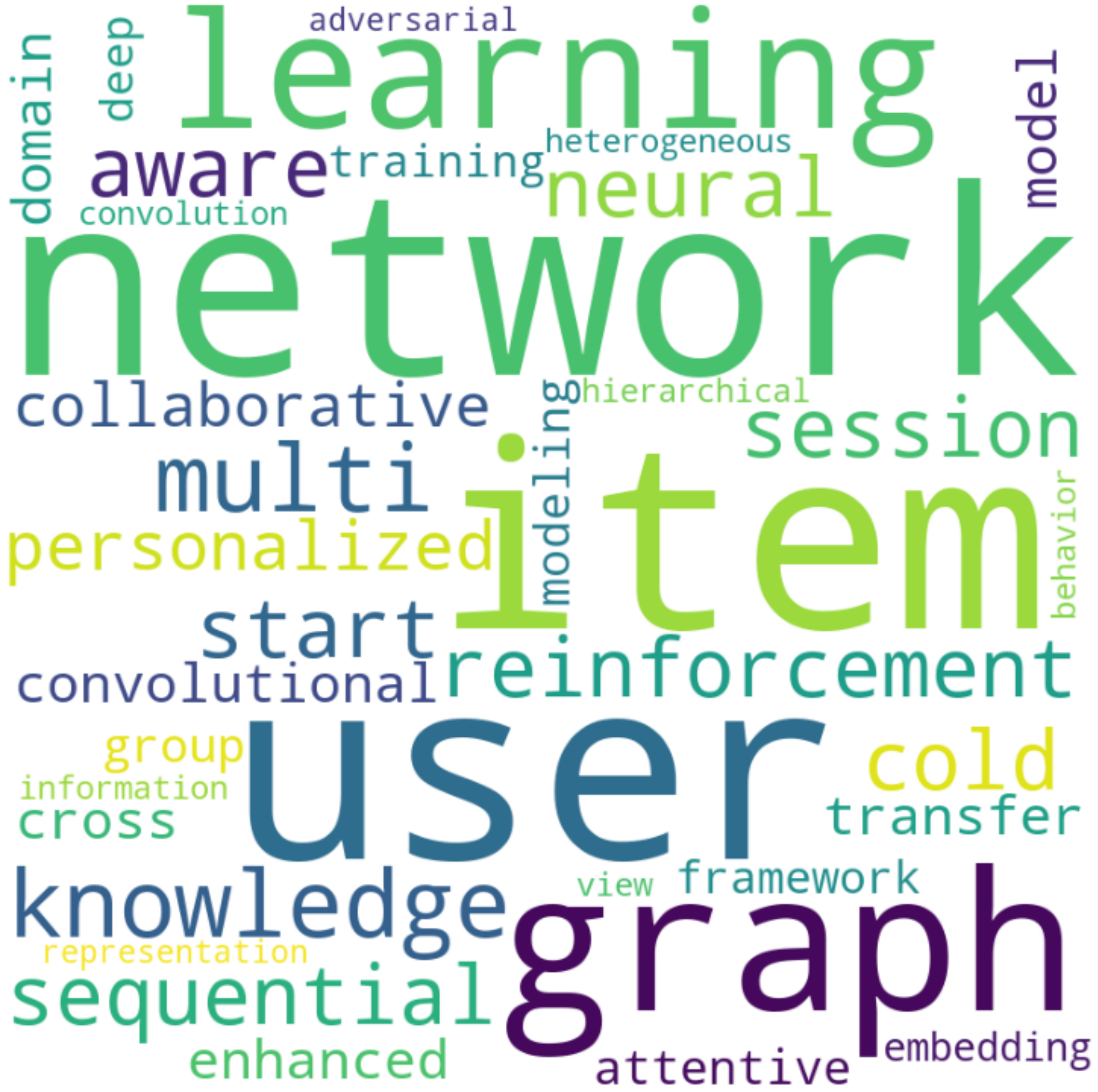
1. Trend

SIGIR 2020 ACCEPTED PAPERS



Ctrl+F: 'recommend'

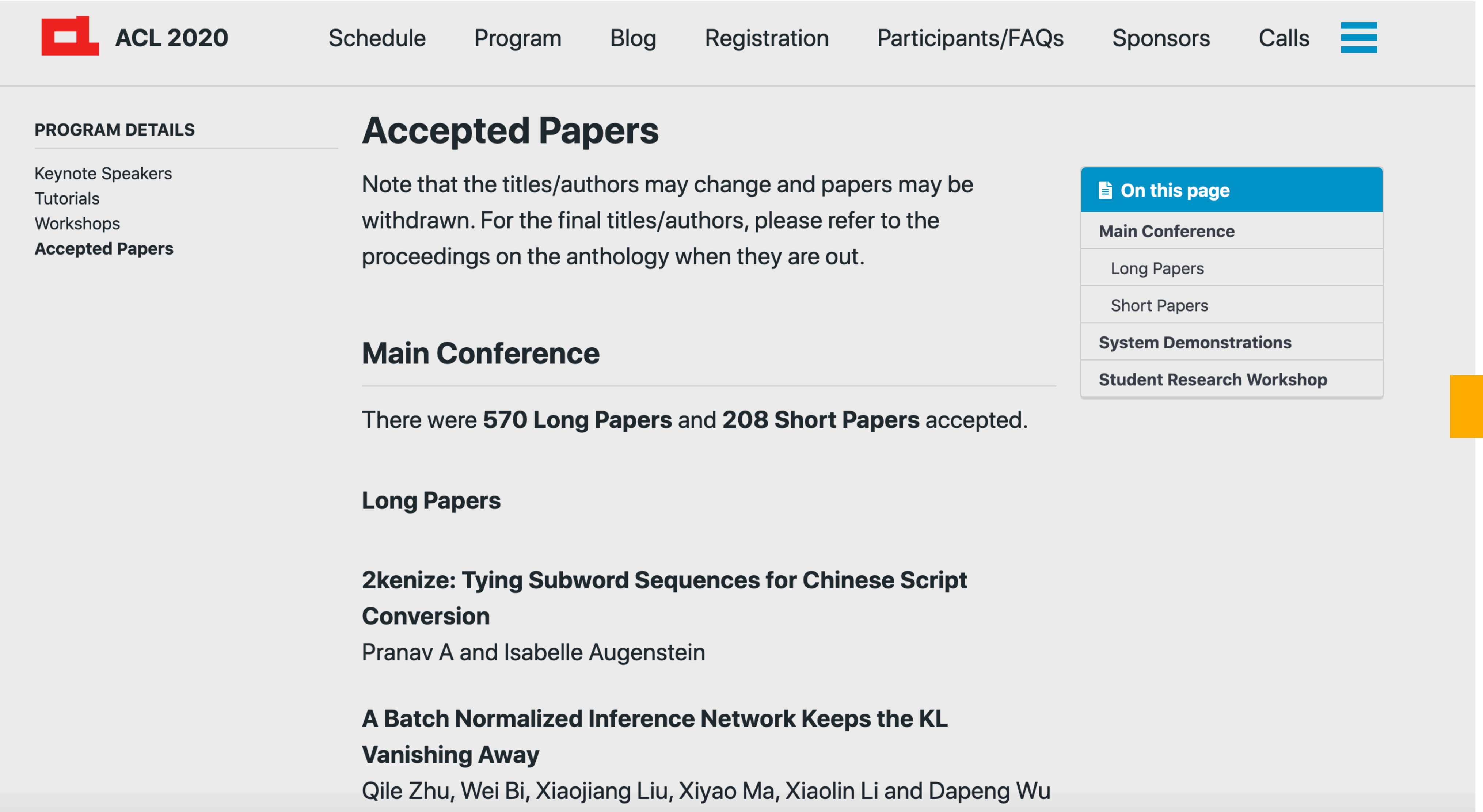
	page	count
0	graph	21
1	learning	18
2	network	18
3	knowledge	11
4	multi	9
5	item	9
6	sequential	9
7	cold	8
8	start	8
9	aware	7
10	neural	7
11	session	7
12	reinforcement	7
13	personalized	6
14	user	6
15	users	6
16	collaborative	5
17	convolutional	5
18	transfer	5
19	cross	5
20	domain	5
21	enhanced	4
22	model	4
23	networks	4
24	attentive	4



'recommendation' 같이 무정보적인 것은 불용어 처리함

1. Trend

ACL 2020 ACCEPTED PAPERS



ACL 2020 Schedule Program Blog Registration Participants/FAQs Sponsors Calls

PROGRAM DETAILS

Keynote Speakers
Tutorials
Workshops
Accepted Papers

Accepted Papers

Note that the titles/authors may change and papers may be withdrawn. For the final titles/authors, please refer to the proceedings on the anthology when they are out.

On this page
Main Conference
Long Papers
Short Papers
System Demonstrations
Student Research Workshop

Main Conference

There were **570 Long Papers** and **208 Short Papers** accepted.

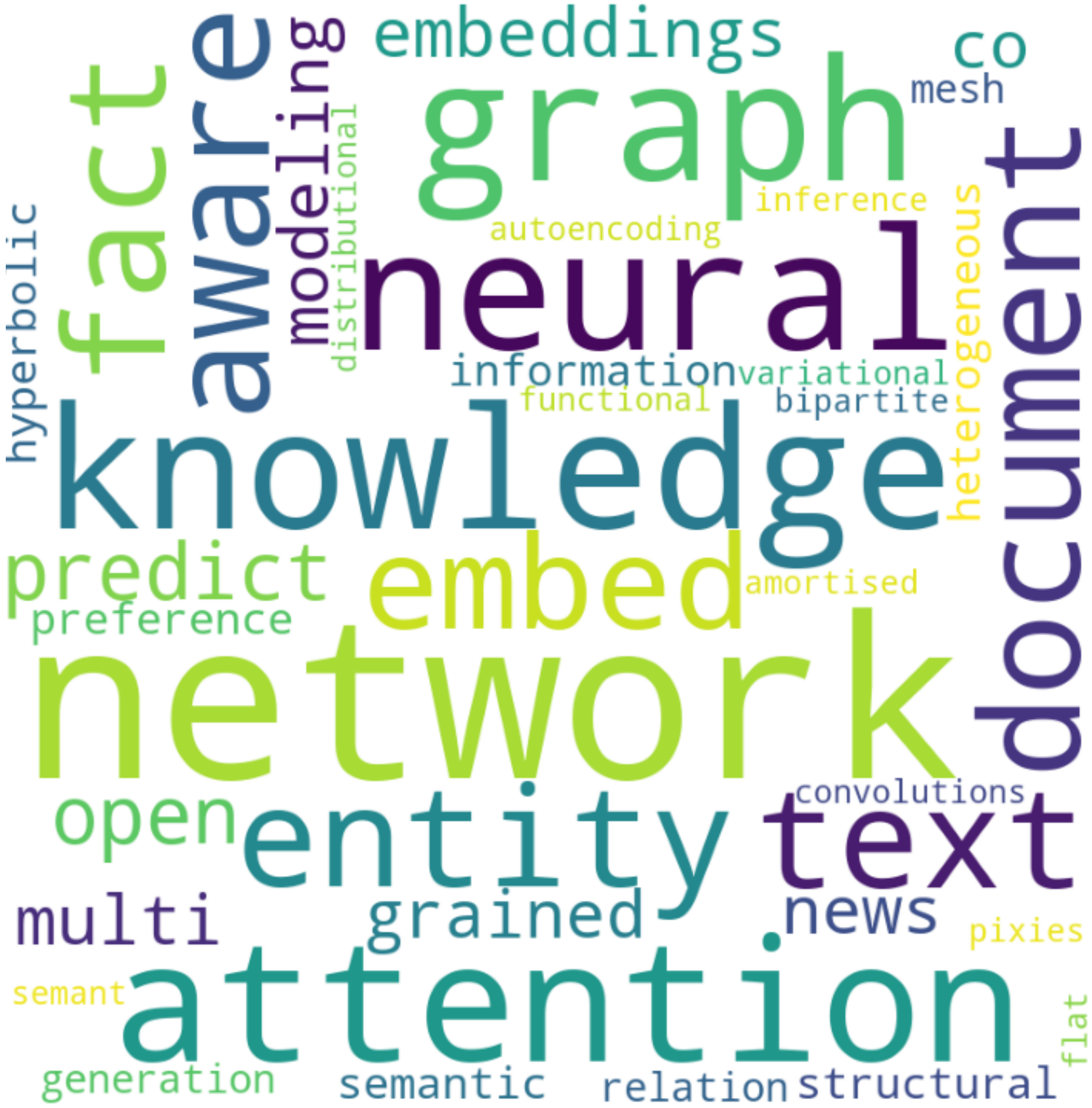
Long Papers

2kenize: Tying Subword Sequences for Chinese Script Conversion
Pranav A and Isabelle Augenstein

A Batch Normalized Inference Network Keeps the KL Vanishing Away
Qile Zhu, Wei Bi, Xiaojiang Liu, Xiyao Ma, Xiaolin Li and Dapeng Wu

Ctrl+F: ‘graph’

	page	count
0	graph	30
1	network	10
2	knowledge	7
3	attention	6
4	networks	5
5	neural	5
6	entity	3
7	document	3
8	fact	3
9	aware	3
10	text	3
11	embed	3
12	predict	2
13	open	2
14	embeddings	2
15	modeling	2
16	multi	2
17	grained	2
18	co	2
19	news	2
20	preference	2



1. Trend

ACL & SIGIR 정리 2020 accepted papers

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0	graph	21
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16	collaborative	5
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18	transfer	5
19	cross	5
20	domain	5
21	enhanced	4
22	model	4
23	networks	4
24	attentive	4

SIGIR

Recommennder System

- Graph는 가장 HOT한 키워드
- 강화학습도 HOT
- Cold Start
- 개인화
- 협업 필터링
- 세션 기반 추천
- 신경망 기반 추천시스템

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ACL

Graph

- GNN으로 NLP 다룸
- Graph Attention Net의 급부상

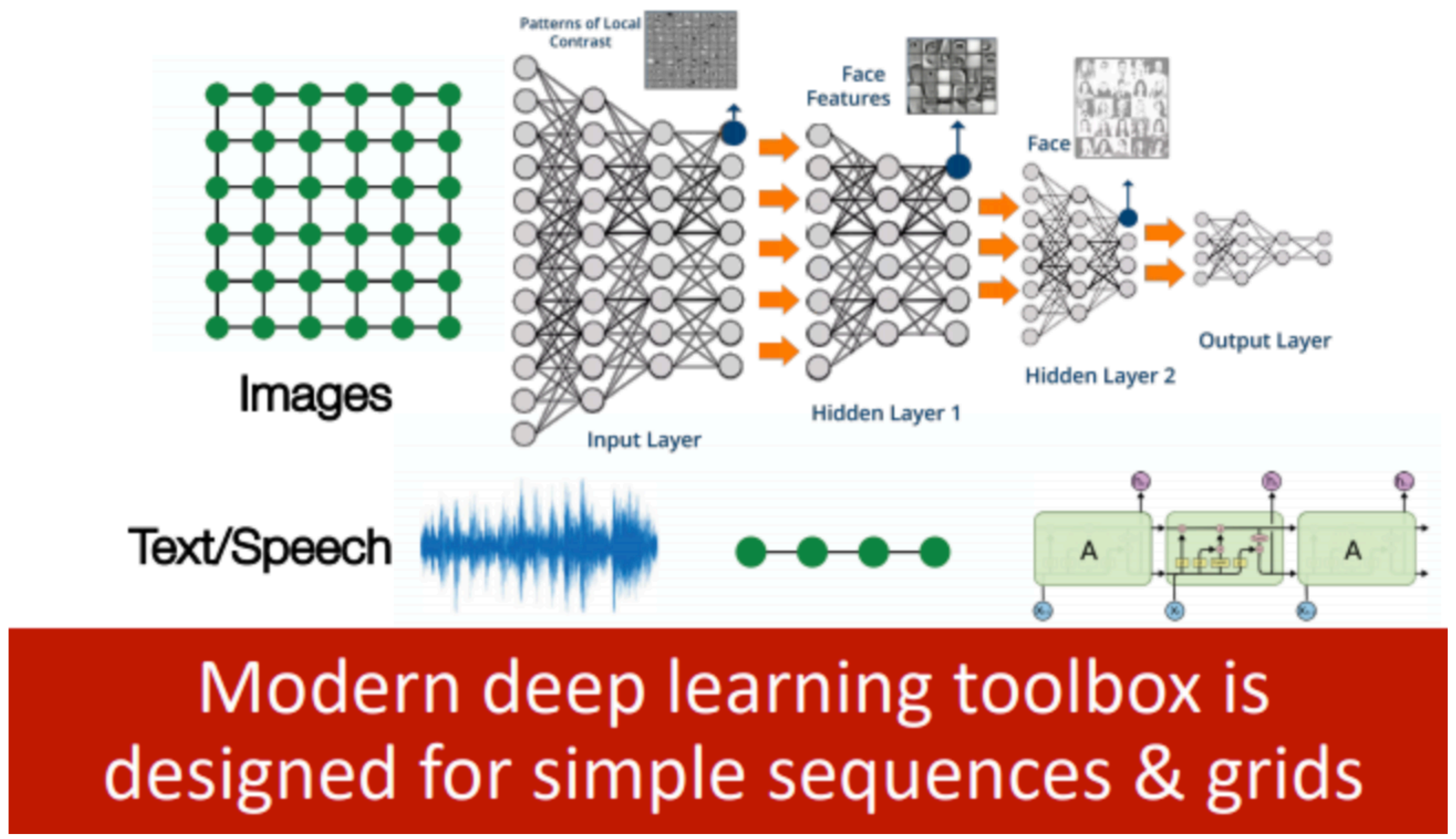
'recommendation' 같이 무정보적인 것은 불용어 처리함

2. Motivation

- 대부분의 성공적인 딥 or 머신러닝 작업에서 사용되던 데이터는 **유클리디안 공간(grid 위에서 표현된 공간)**에서 표현되어지다.

- 하지만 데이터가 비유클리디안 공간에서 만들어지거나 **복잡한 관계를 가진 그래프**로 표현된 경우,
기존의 머신러닝 알고리즘으로 이것을 처리하기 어렵다. (그래프는 비유클리드 공간 위에서 표현됨)

- e-커머스: 구매자와 상품 간의 복잡한 상호관계를 다룬다.
- 화학: 분자들은 그래프로 모델화된다.



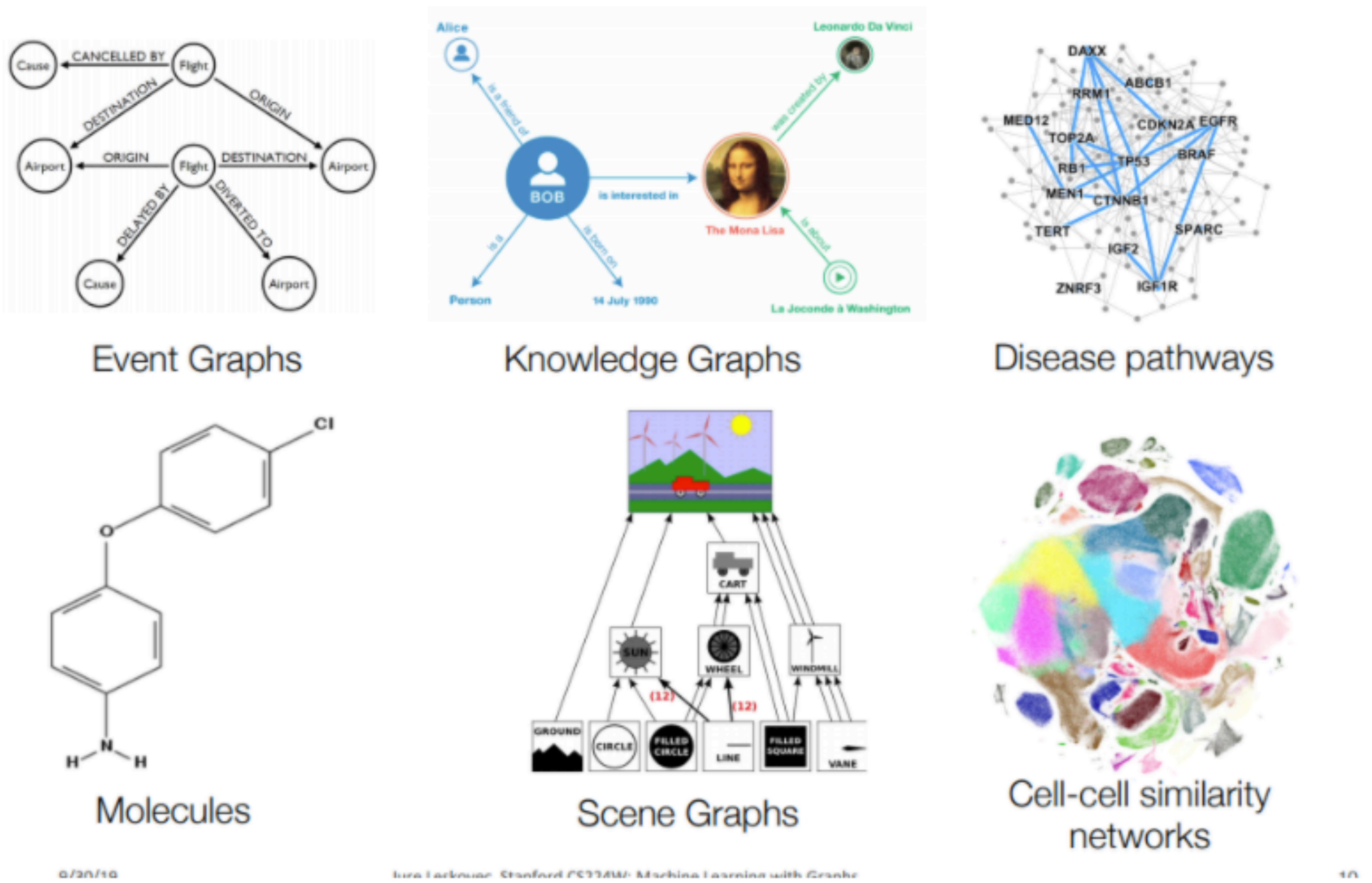
ConvGNNs
컴퓨터 비전에서 CNN의 성공이 동기가 되어, 그래프 데이터의. Convolution 개념에 대한 재정의가 이루어졌다.
- the spectral-based approaches (Bruna et al 2013)
- The spatial-based approaches

Reccurent GNNs

AutoEncoder GNNs

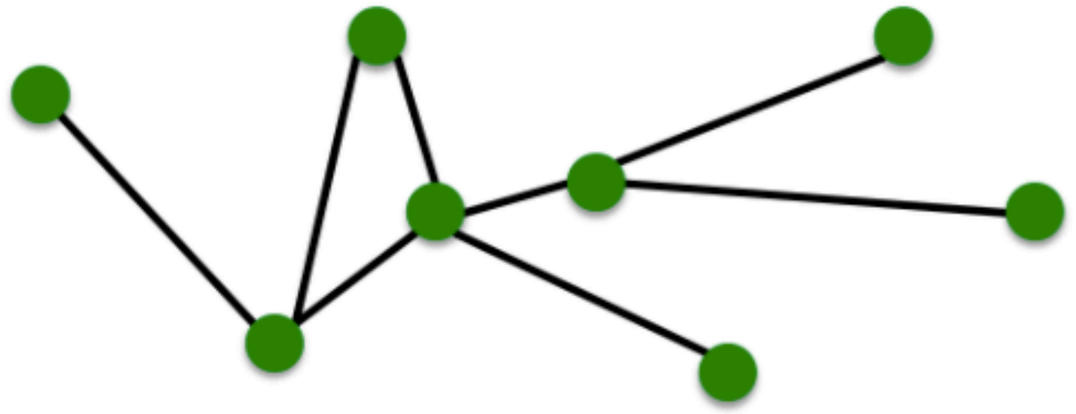
Graph Attention Networks

...

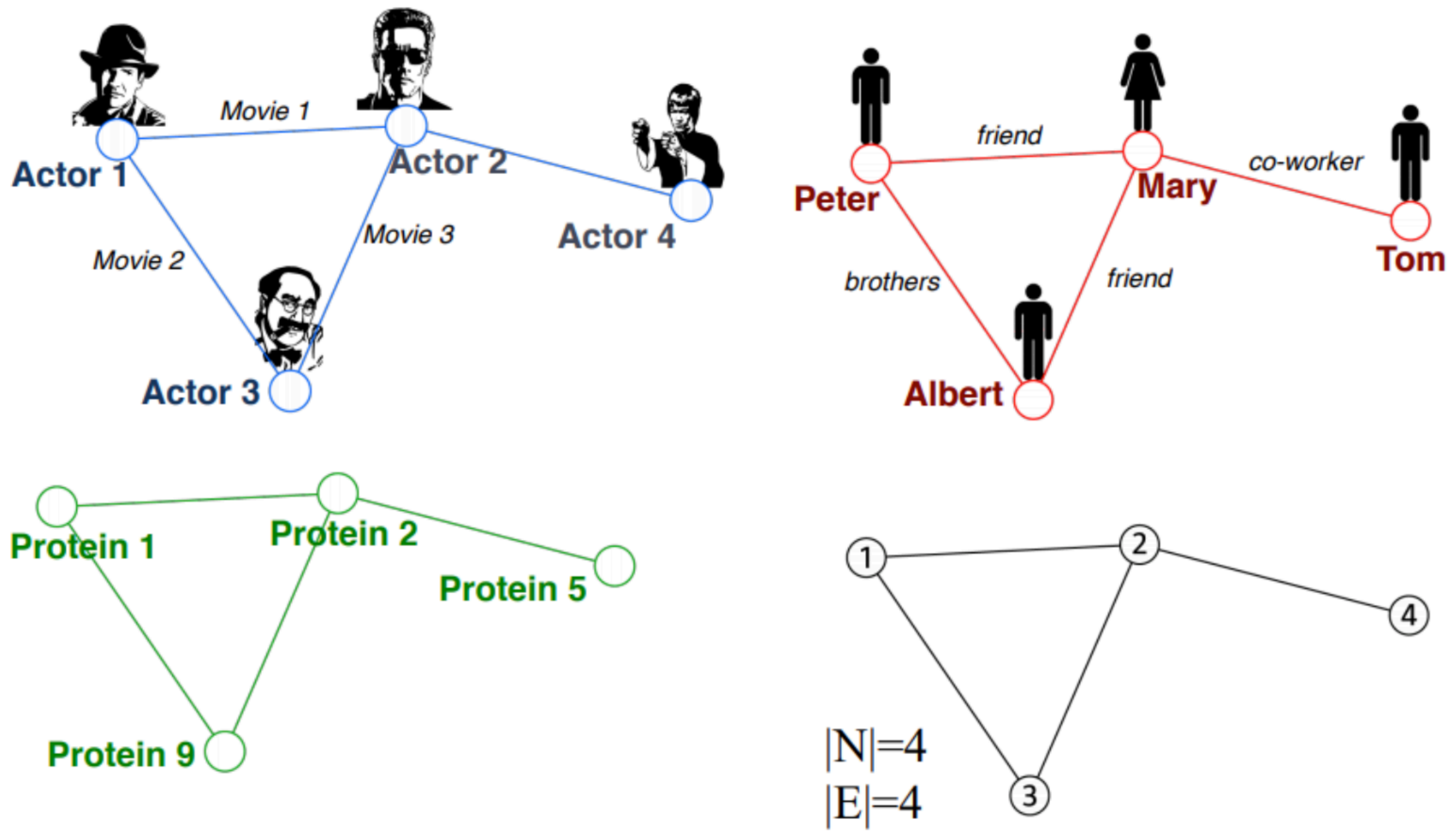


3. Graph

3.1 Def

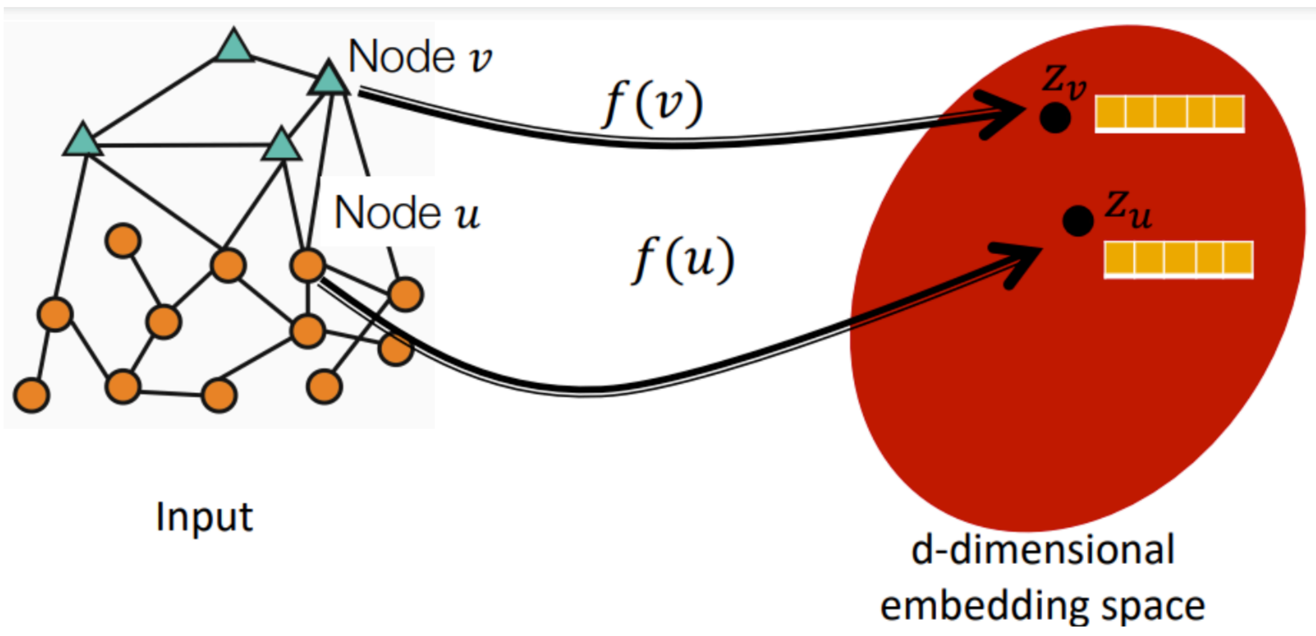


- **Objects:** nodes, vertices N
- **Interactions:** links, edges E
- **System:** network, graph $G(N,E)$



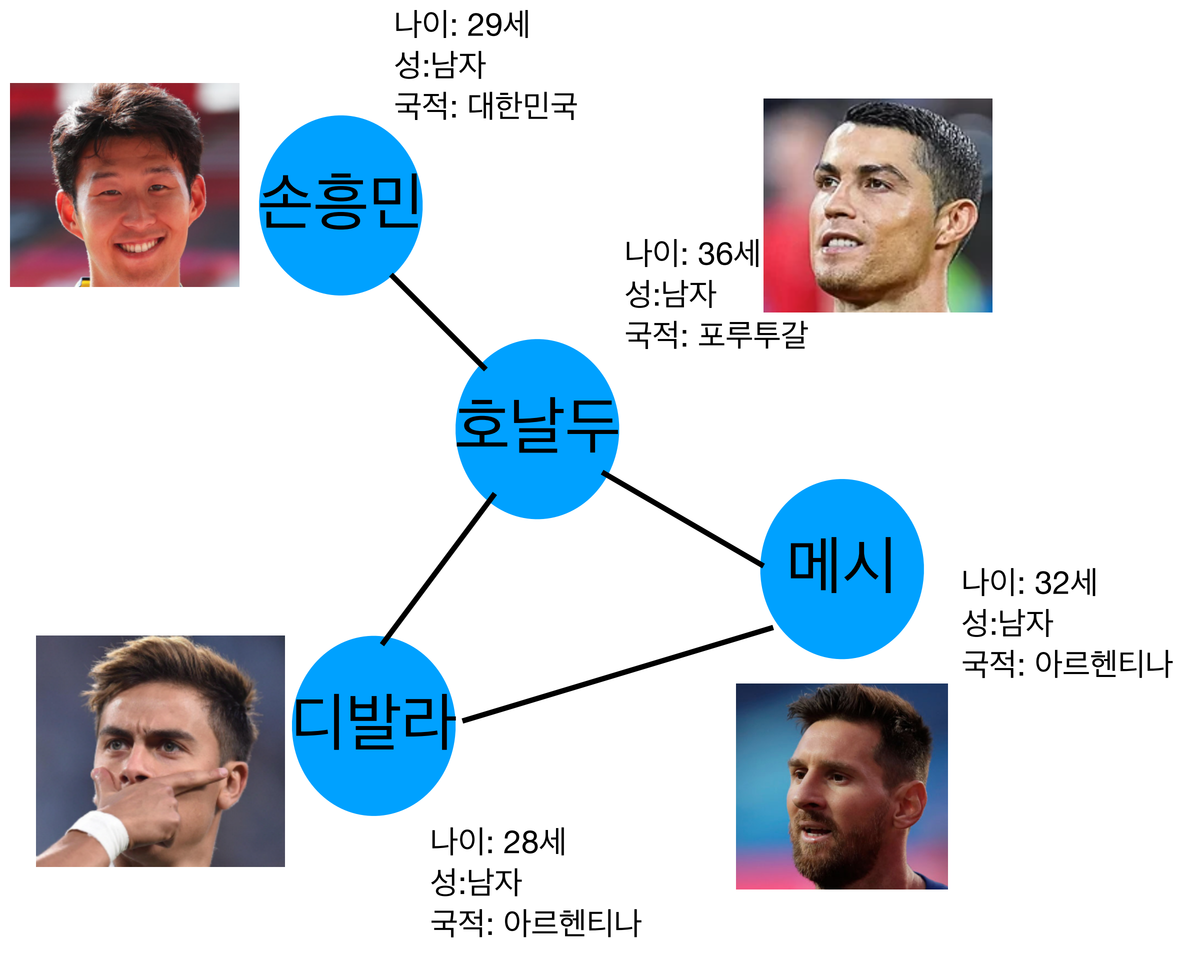
3.2 Embedding Node

그래프의 node를 d 차원으로 임베딩. 여기서 유사한 이웃을 가진 노드들은 서로 가까이 있게끔 임베딩된다.



3. Graph

3.3 How to represent graph into the matrix



	Feature1	Feature2	Feature3	국적을 나타내는 Features라고 해보자
son	0	1	0	대한민국
Ronaldo	0	1	1	포르투갈
Messi	1	1	1	둘다 아르헨티나
Dybala	1	1	1	

N(node) x F(features)의 **Node Feature Matrix** X_{ij}

	son	Ronaldo	Messi	Dybala
son	0	1	0	0
Ronaldo	1	0	1	1
Messi	0	1	0	1
Dybala	0	1	1	0

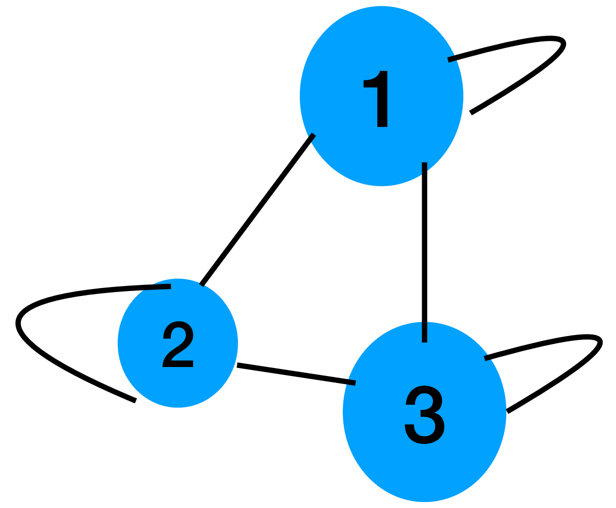
N x N(node)의 **Adjacent Matrix** A_{ij}

	son	Ronaldo	Messi	Dybala
son	1	0	0	0
Ronaldo	0	3	0	0
Messi	0	0	2	0
Dybala	0	0	0	2

D Degree matrix

참고: [#30.Lec] Basic of Graph Convolution Network - 딥러닝 홀로서기

4. Graph Convolutional Networks



4.1 The limits of adjacent matrix

1) 각 노드 자신에 대한 정보가 학습 시 업데이트되지 않는다.

→ 각 Mat에 I를 더해줌으로써, 각 노드 자기 자신에 대한 정보도 학습 시 업데이트할 수 있다.

	son	Ronaldo	Messi	Dybala
son	1	0	0	0
Ronaldo	0	3	0	0
Messi	0	0	2	0
Dybala	0	0	0	2

D Degree matrix

\+

	son	Ronaldo	Messi	Dybala
son	1	0	0	0
Ronaldo	0	1	0	0
Messi	0	0	1	0
Dybala	0	0	0	1

I

=

2	0	0	0
0	4	0	0
0	0	3	0
0	0	0	3

$\tilde{D}$

	son	Ronaldo	Messi	Dybala
son	0	1	0	0
Ronaldo	1	0	1	1
Messi	0	1	0	1
Dybala	0	1	1	0

A_{ij} Adjacent Matrix

\+

	son	Ronaldo	Messi	Dybala
son	1	0	0	0
Ronaldo	0	1	0	0
Messi	0	0	1	0
Dybala	0	0	0	1

I

=

1	1	0	0
1	1	1	1
0	1	1	1
0	1	1	1

$\tilde{A}_{ij}$

4. Graph Convolutional Networks

4.1 The limits of adjacent matrix

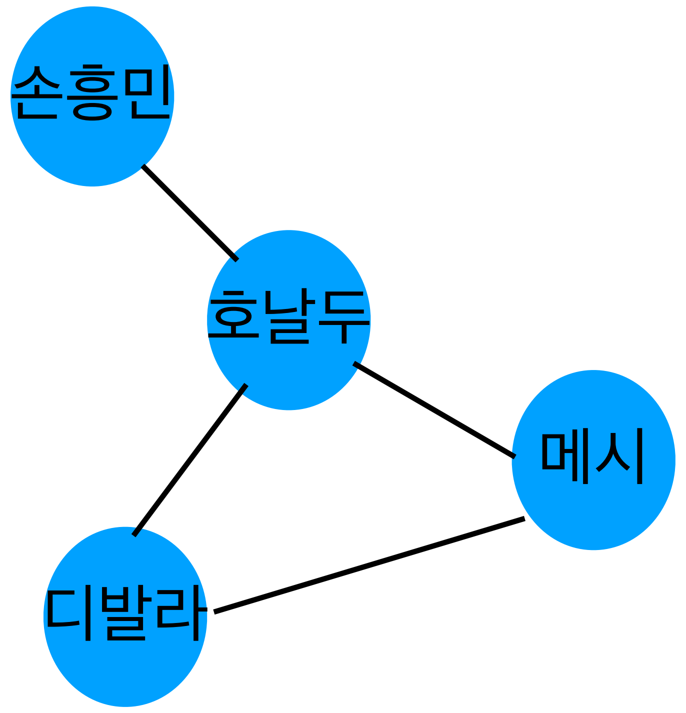
2) 기본적인 인접행렬 A는 정규화가 되어있지 않아 gradient explosion을 발생시키거나 feature matrix와 곱할 때(AX) X의 크기를 불안정하게 크게 만들 수 있다.

해소방안: $\tilde{A} \longrightarrow \hat{A} = D^{\tilde{-}0.5}\tilde{A}D^{\tilde{-}0.5}$

4. Graph Convolutional Networks

4.1 The limits of adjacent matrix

2) 기본적인 인접행렬 A는 정규화가 되어있지 않아 gradinet explosion을 발생시키거나 feature matrix와 곱할 때(AX) X의 크기를 불안정하게 크게 만들 수 있다.



2	0	0	0
0	4	0	0
0	0	3	0
0	0	0	3

$\tilde{D}$

→

1/2	0	0	0
0	1/4	0	0
0	0	1/3	0
0	0	0	1/3

$\tilde{D}^{-1}$

평균으로 정규화

1/2	0	0	0
0	1/4	0	0
0	0	1/3	0
0	0	0	1/3

$\tilde{D}^{-1}$

*

1	1	0	0
1	1	1	1
0	1	1	1
0	1	1	1

$\tilde{A}_{ij}$

→

1/2	1/2	0	0
1/4	1/4	1/4	1/4
0	1/3	1/3	1/3
0	1/3	1/3	1/3

S

고차 노드에 더 작은 수를 곱함으로써 영향력을 줄이기

*

1/2	0	0	0
0	1/4	0	0
0	0	1/3	0
0	0	0	1/3

$\tilde{D}^{-1}$

=

1/2	1/8	0	0
1/8	1/16	1/12	1/12
0	1/12	1/9	1/9
0	1/12	1/9	1/9

$\hat{A}$

4. Graph Convolutional Networks

4.1 The limits of adjacent matrix

2	0	0	0
0	4	0	0
0	0	3	0
0	0	0	3

$\tilde{D}$

1	1	0	0
1	1	1	1
0	1	1	1
0	1	1	1

$\tilde{A}_{ij}$

$$\hat{A} = \tilde{D}^{-1}\tilde{A}\tilde{D}^{-1}$$

이 같은 계산은 사실상 정규화를 두 번 하는 것이기 때문에   아래 같이 수정함으로써 rebalance 해주기

$$\downarrow$$

$$\hat{A} = \tilde{D}^{-0.5}\tilde{A}\tilde{D}^{-0.5}$$

Normalized Adjacency Matrix $\longrightarrow$

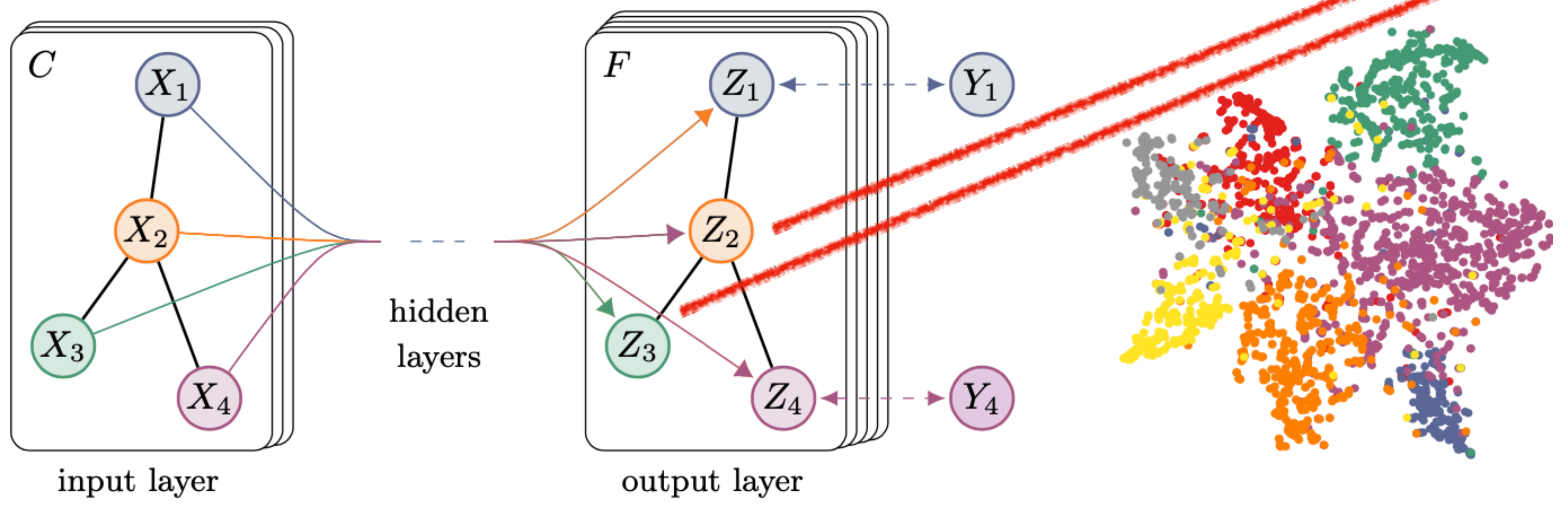
$$H^{(l+1)} = \sigma\left(\underbrace{\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}}_{=\hat{A}}H^{(l)}W^{(l)}\right).$$

- H: node feature matrix
- W: weight

4. Graph Convolutional Networks

we consider a two-layer GCN for semi-supervised node classification on a graph with a symmetric adjacency matrix A

라벨이 없는 것도 분류를 한다는 점에서 준지도학습을 잘 수행



(a) Graph Convolutional Network (b) Hidden layer activations

$$\hat{A} = \tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}$$

$$Z = f(X, A) = \mathrm{softmax}\left(\hat{A}\ \mathrm{ReLU}\left(\hat{A}XW^{(0)}\right)W^{(1)}\right)$$

Layer1

Layer2

$$\mathcal{L} = -\sum_{l\in\mathcal{Y}_L}\sum_{f=1}^{F} Y_{lf}\ln Z_{lf}\,,$$

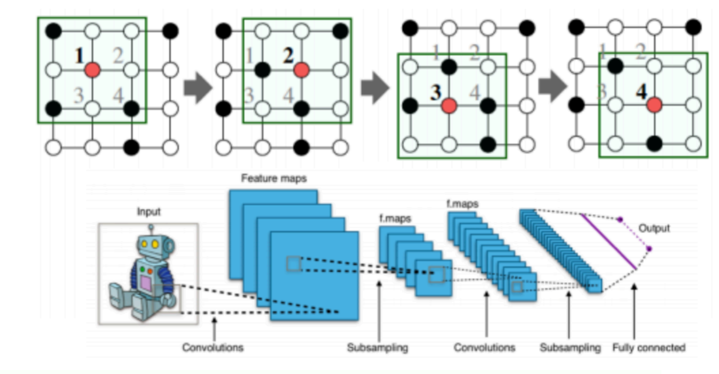
Y: 실제 값, Z: 예측 값: Y,Z의 크로스엔트로피

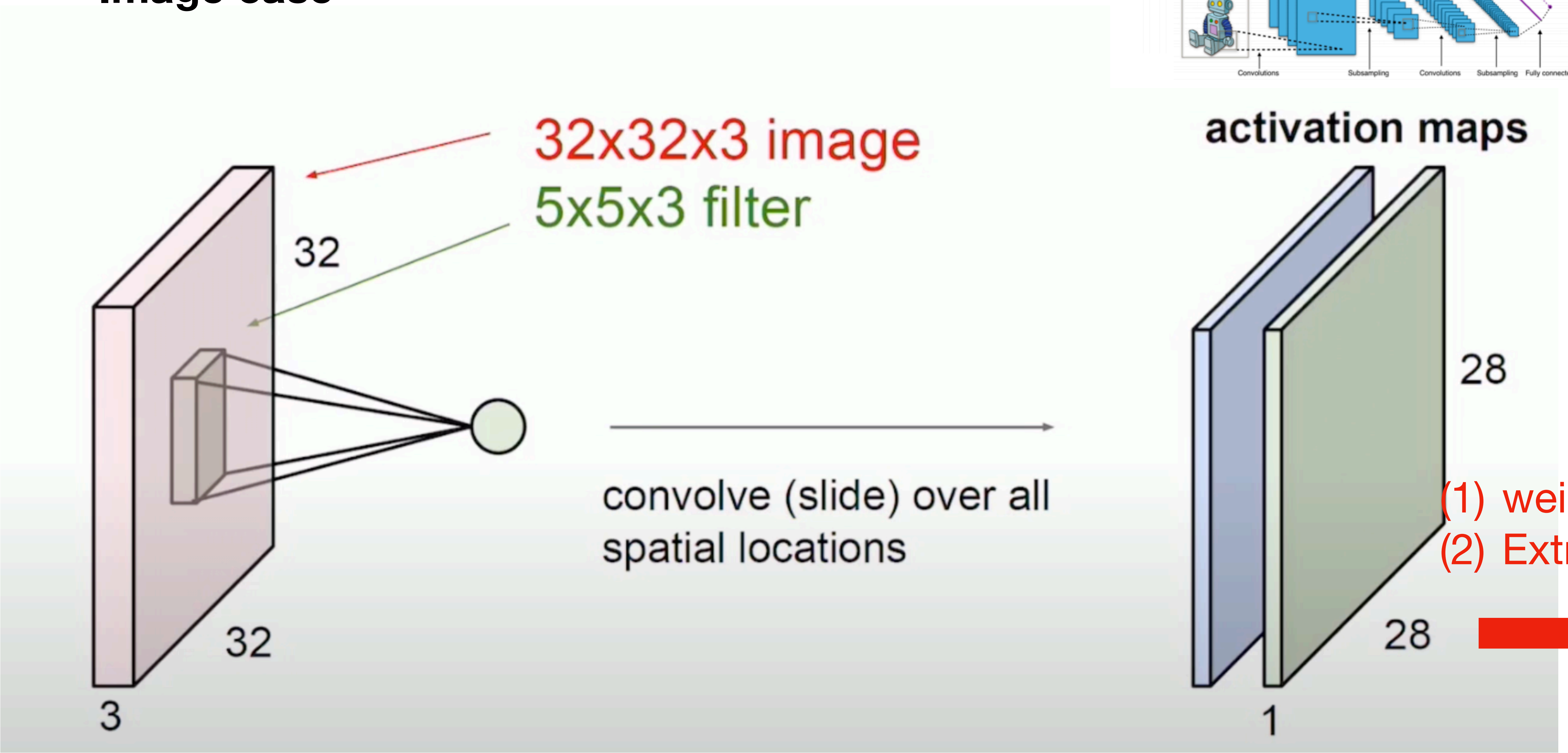
4. Graph Convolutional Networks

4.1 Convolution

Image case

CNN on an image:



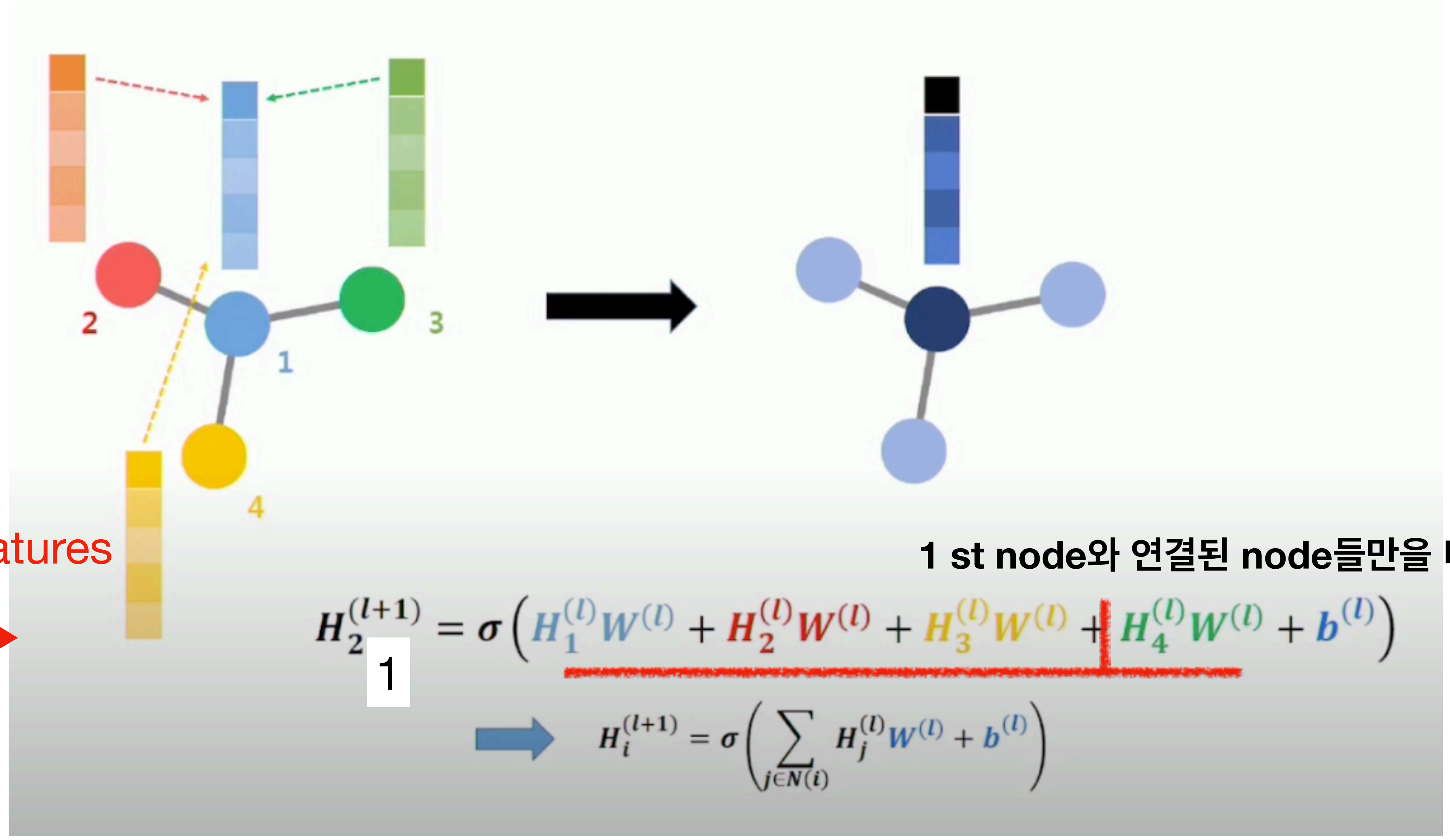


(1) weight sharing
(2) Extracting local features

- Filter: 한 층 당 25 개의 파라미터. 3 개의 층이니까 75 개 파라미터가 있다
- 저 Filter는 정해진 stride 만큼 건너 뛰면서 전체 image를 조사
- 몇 개의 필터를 사용했는가에 따라 activation map의 depth 결정된다

- **UPDATE:** Conv를 하나 거칠 때 마다 (**이미지**의 특성을 담고 있는) activation map의 값이 업데이트

Graph case



1 st node와 연결된 node들만을 더해줌

- **W**: Weight
- **H**: node feature matrix
- H_n: n th node의 feature 값들
- l: l th layer

- **UPDATE:** Conv를 하나 거칠 때 마다 (**노드**의 특성을 담고 있는) activation map의 값이 업데이트

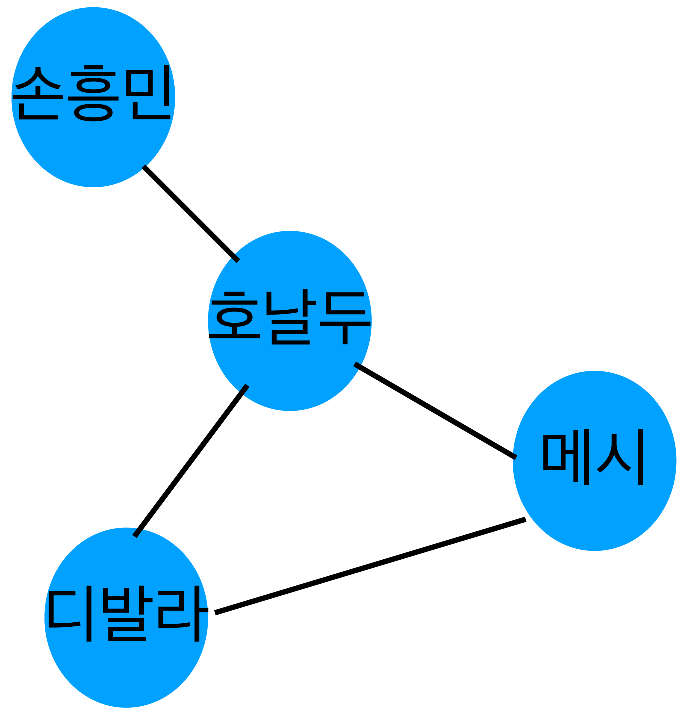
4. Graph Convolutional Networks

4.2 Compact Forms

$$H_i^{(l+1)} = \sigma\left(\sum_{j \in N(i)} H_j^{(l)} W^{(l)} + b^{(l)}\right) \longrightarrow H^{(l+1)} = \sigma\left(AH^{(l)} W^{(l)} + b^{(l)}\right)$$

Adjacent Matrix

learnable parameters are shared



	son	Ronaldo	Messi	Dybala
son	1/2	1/8	0	0
Ronaldo	1/8	1/16	1/12	1/12
Messi	0	1/12	1/9	1/9
Dybala	0	1/12	1/9	1/9

Normalized
Adjacent Matrix
(Ahat 4,4)

	feature 1	Feature 2	Feature 3	feature 4	Feature 5
son	1	1	1	0	1
Ronaldo	1	0	1	1	0
Messi	0	1	1	1	1
Dybala	0	1	1	1	1

Node feature Matrix
(X 4,5)

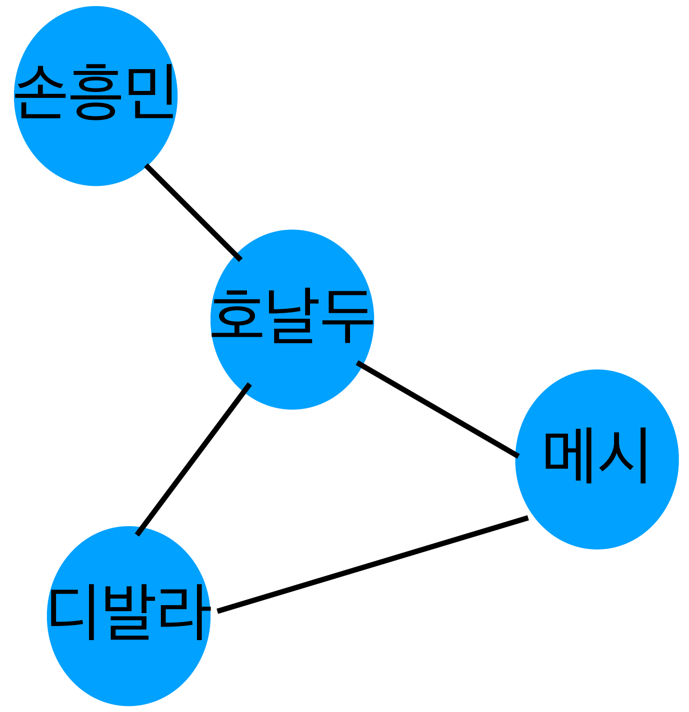
	Filter1	Filter2	…	Filter64
feature1	1	1	1	0
Feature2	1	0	1	1
Feature3	0	1	1	1
Feature4	0	1	1	1
Feature5	1	1	0	1

Weight
(W 5,64)

자기 자신과는 연결되어 있지는 않지만, 이전 레이어에서 다음 레이어로 갈 때, 다음 레이어에서 이전 것의 정보를 받아야 하니까 자기 자신은 1로 가정

4. Graph Convolutional Networks

4.2 Compact Forms



	feature 1	Feature 2	Feature 3	feature 4	Feature 5
son	1	1	1	0	1
Ronaldo	1	0	1	1	0
Messi	0	1	1	1	1
Dybala	0	1	1	1	1

Node feature Matrix (X 4,5)

*

	Filter1	Filter2	...	Filter64
feature1	1	1	1	0
Feature2	1	0	1	1
Feature3	0	1	1	1
Feature4	0	1	1	1
Feature5	1	1	0	1

Weight (W 5,64)

σ (

	son	Ronaldo	Messi	Dybala
son	1/2	1/8	0	0
Ronaldo	1/8	1/16	1/12	1/12
Messi	0	1/12	1/9	1/9
Dybala	0	1/12	1/9	1/9

Ahat(4,4)

	Filter1	Filter2	…	Filter64
son	1	1	1	1
Ronaldo	1	1	0	1
Messi	0	1	0	1
Dybala	0	1	0	1

XW (4,64) 각 노드의 고차원 정보를 담은 행렬

)

$$H^{(l+1)} = \sigma\left(AH^{(l)}W^{(l)} + b^{(l)}\right)$$

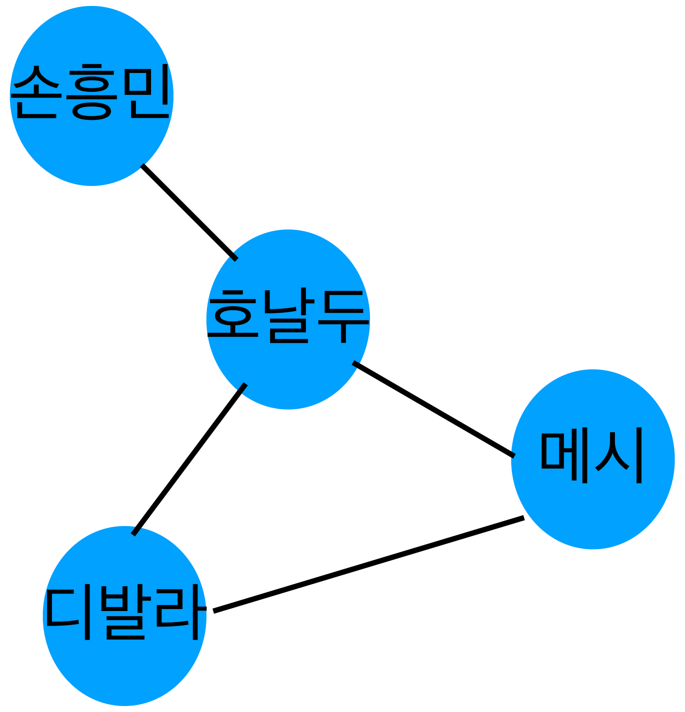
learnable parameters are shared

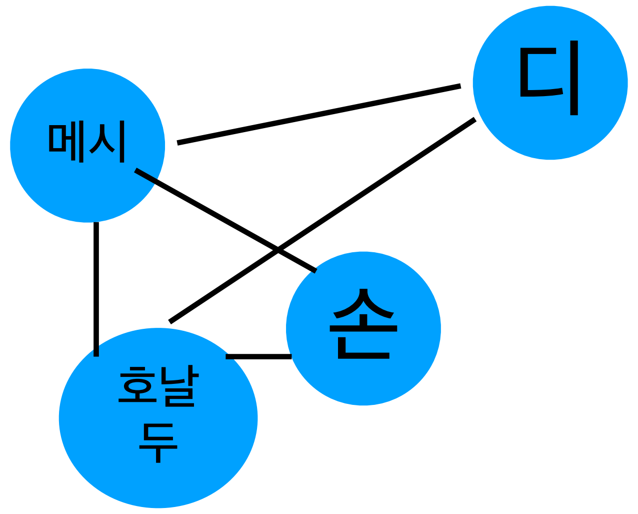
4. Graph Convolutional Networks

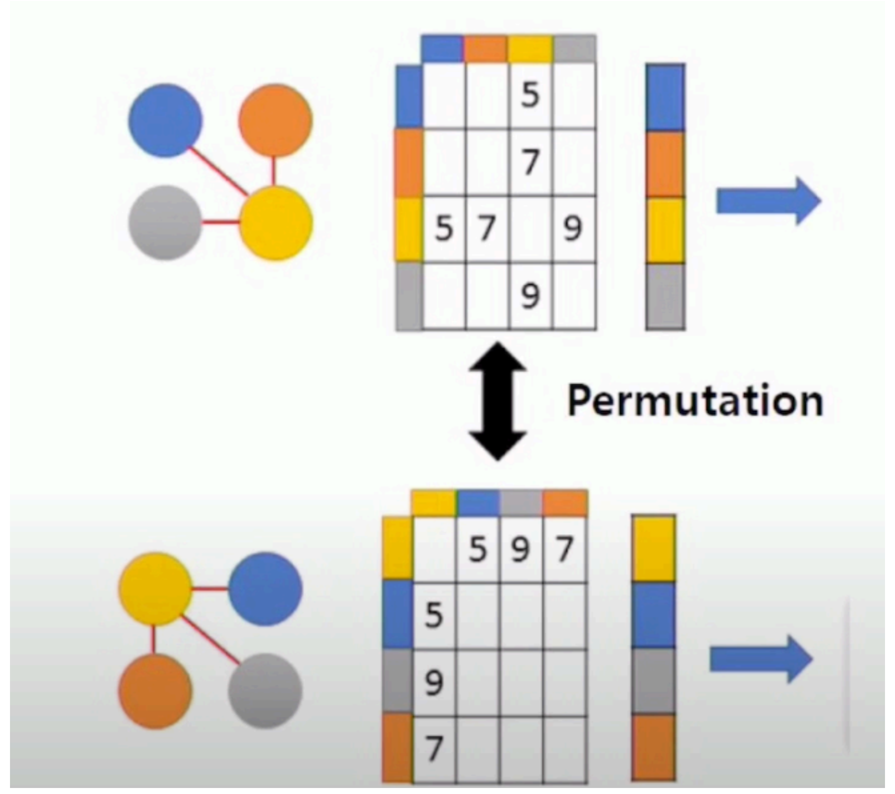
4.3 Readout Layer

Permutation Invariance

Pytorch-geometric
stellargraph

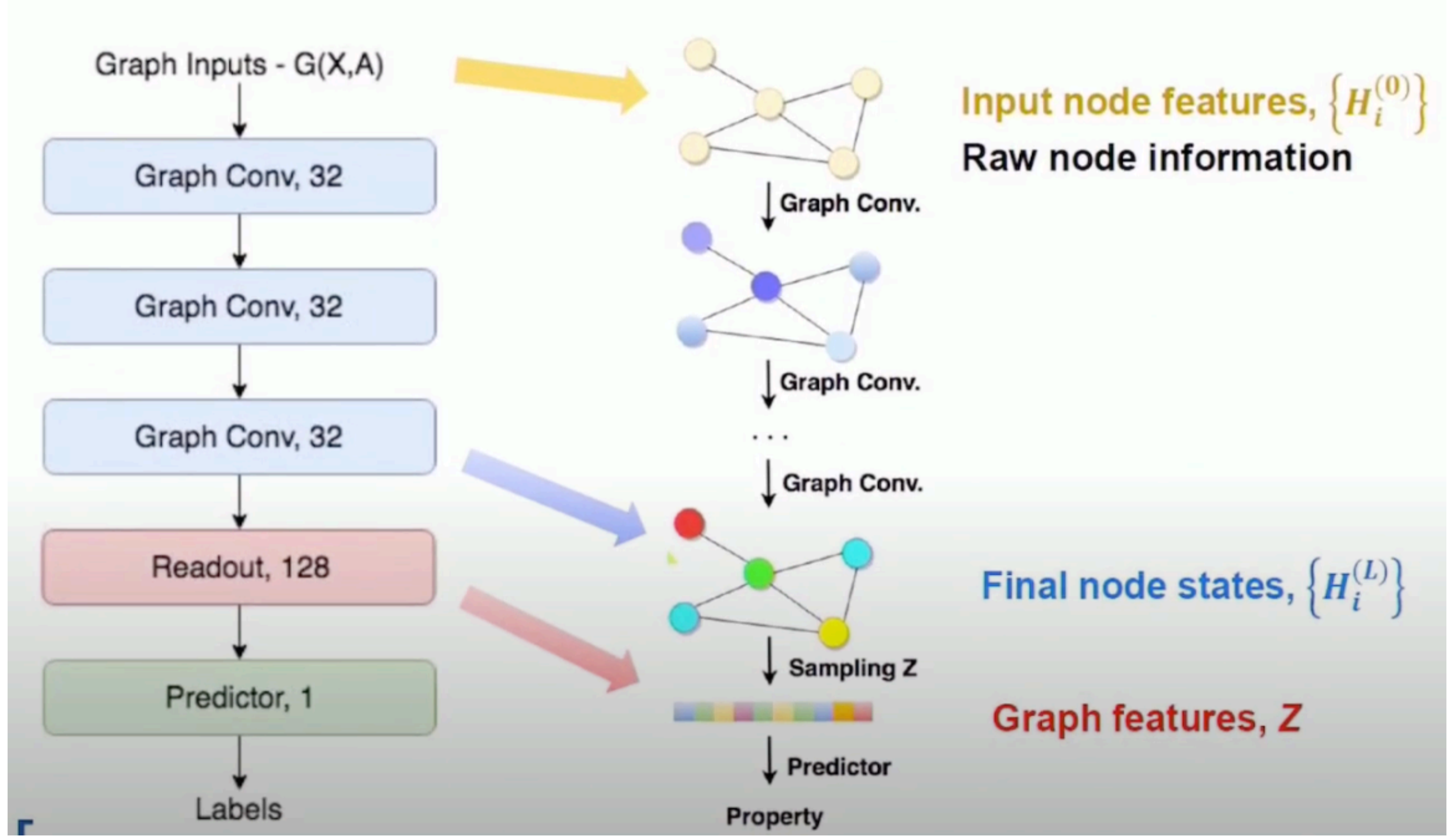






Node-wise summation

$$z_G = \tau\left(\sum_{i \in G} MLP\left(H_i^{(L)}\right)\right)$$



- 노드의 순서가 바뀐다고 해서 그래프가 바뀌지는 않는다.
- 하지만 우리가 표현하는 **node feature matrix**는 그래프 모양이 바뀜에 따라 달라진다.
- 이것에 invariance를 부여하기 위해 readout layer를 거친다.

	Feature1	Feature2	Feature3
son	0	1	0
Ronaldo	0	1	1
Messi	1	1	1
Dybala	1	1	1

→

	Feature1	Feature2	Feature3
Ronaldo	0	1	1
son	0	1	1
Messi	1	1	1
Dybala	1	1	1

5. Experiments

Table 1: Dataset statistics, as reported in Yang et al. (2016).

Dataset	Type	Nodes	Edges	Classes	Features	Label rate
Citeseer	Citation network	3,327	4,732	6	3,703	0.036
Cora	Citation network	2,708	5,429	7	1,433	0.052
Pubmed	Citation network	19,717	44,338	3	500	0.003
NELL	Knowledge graph	65,755	266,144	210	5,414	0.001

Table 2: Summary of results in terms of classification accuracy (in percent).

Method	Citeseer	Cora	Pubmed	NELL
ManiReg [3]	60.1	59.5	70.7	21.8
SemiEmb [28]	59.6	59.0	71.1	26.7
LP [32]	45.3	68.0	63.0	26.5
DeepWalk [22]	43.2	67.2	65.3	58.1
ICA [18]	69.1	75.1	73.9	23.1
Planetoid* [29]	64.7 (26s)	75.7 (13s)	77.2 (25s)	61.9 (185s)
GCN (this paper)	**70.3** (7s)	**81.5** (4s)	**79.0** (38s)	**66.0** (48s)
GCN (rand. splits)	67.9 ± 0.5	80.1 ± 0.5	78.9 ± 0.7	58.4 ± 1.7

References

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