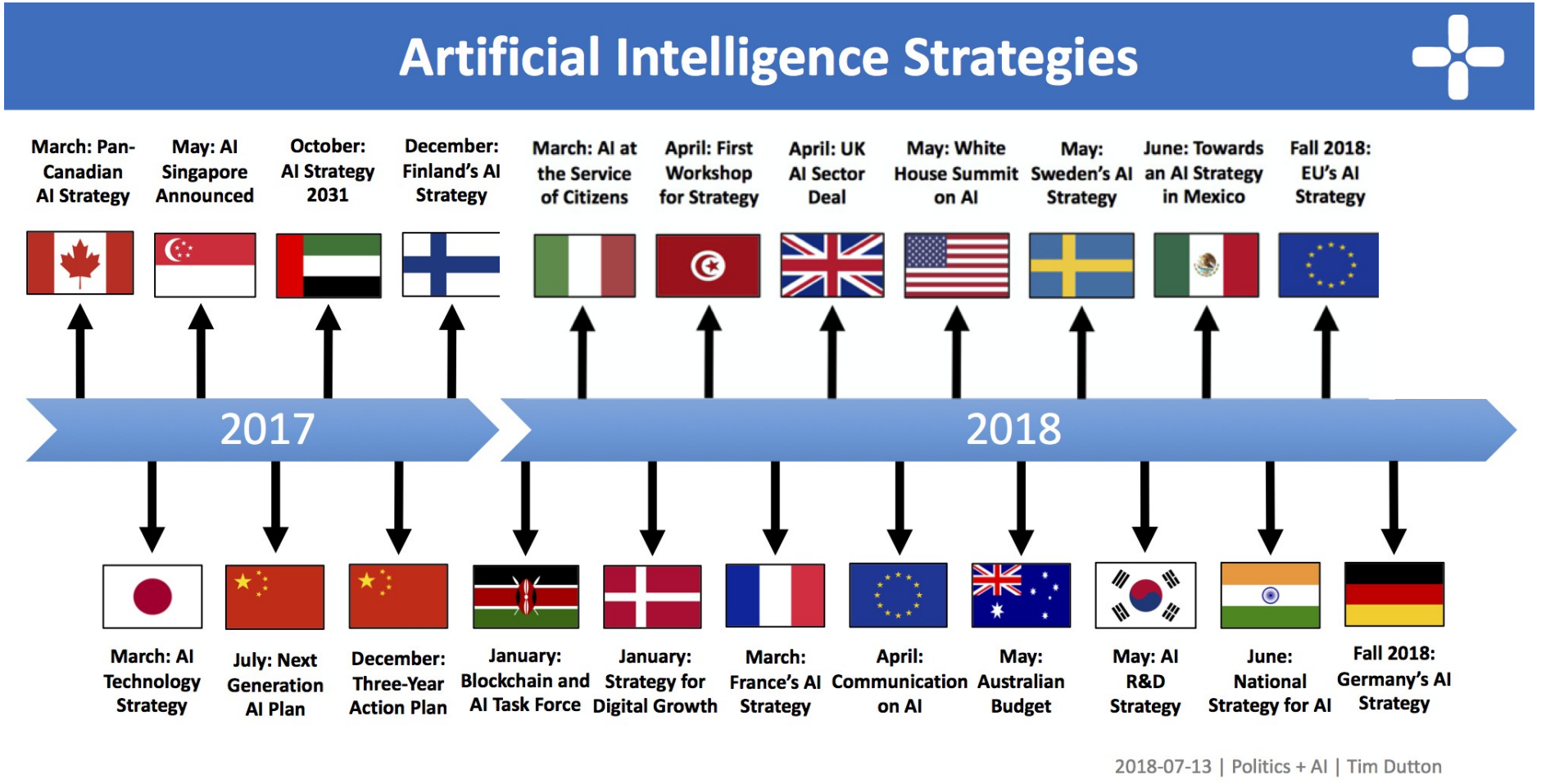
图神经网络及认知推理

Jie Tang
Computer Science
Tsinghua University

The slides can be downloaded at http://keg.cs.tsinghua.edu.cn/jietang

人工智能的第三次浪潮


Artificial Intelligence Strategies
March: Pan-Canadian AI Strategy
May: AI Singapore Announced
October: AI Strategy 2031
December: Finland's AI Strategy
March: AI at the Service of Citizens
April: First Workshop for Strategy
April: UK AI Sector Deal
May: White House Summit on AI
May: Sweden's AI Strategy
June: Towards an AI Strategy in Mexico
Fall 2018: EU's AI Strategy
2017
2018
March: AI Technology Strategy
July: Next Generation AI Plan
December: Three-Year Action Plan
January: Blockchain and AI Task Force
January: Strategy for Digital Growth
March: France's AI Strategy
April: Communication on AI
May: Australian Budget
May: AI R&D Strategy
June: National Strategy for AI
Fall 2018: Germany's AI Strategy
2018-07-13 | Politics + AI | Tim Dutton

Artificial Intelligence

AlphaGo

Self-driving

- dog + cat =

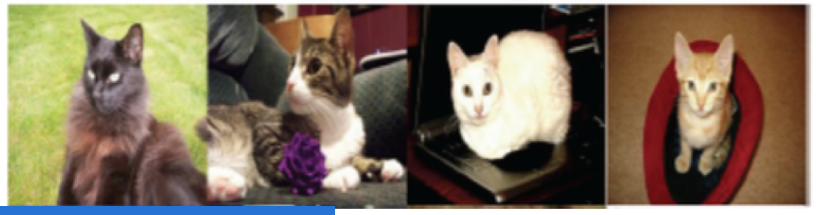
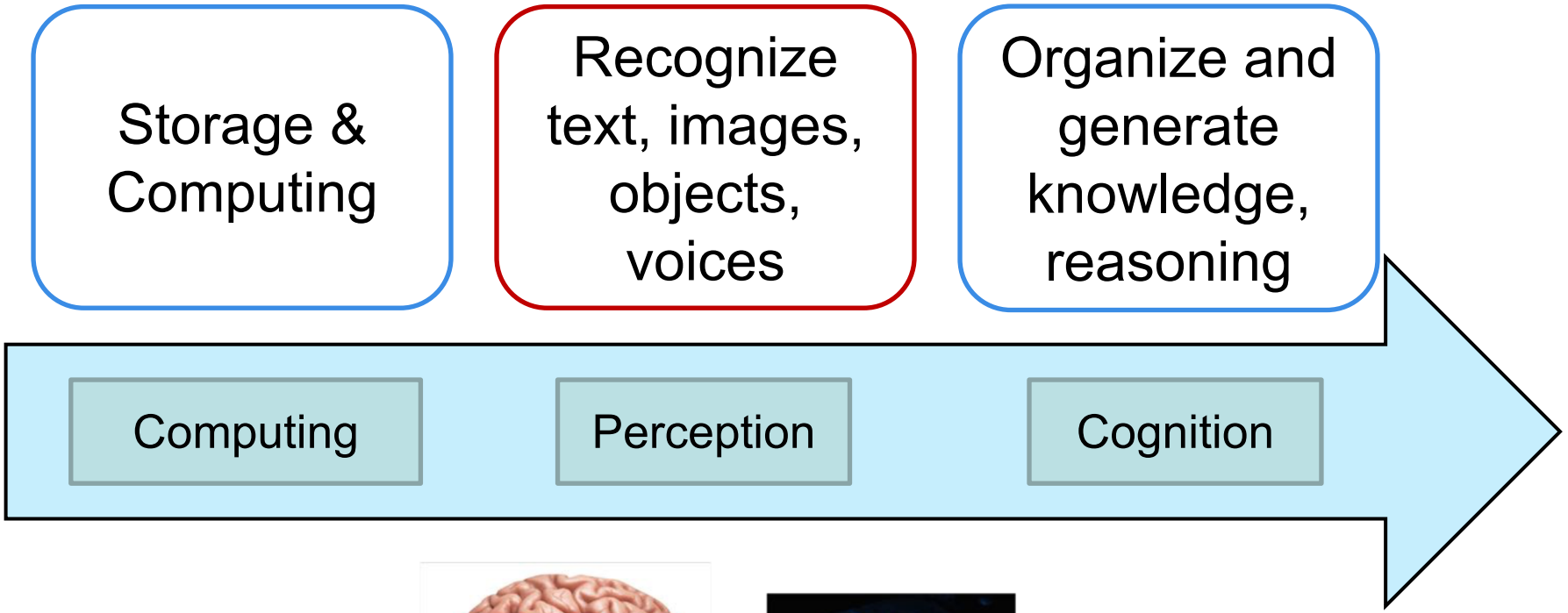


Image recognition

AI趋势：从感知到认知

- From perceptron to cognition



Stochastic vs Deterministic

Uncertainty!

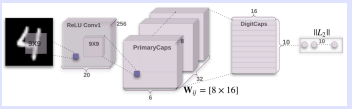
算法

Frank Rosenblatt
Cornell University
psychologist

Geoffery Hinton
University of Toronto
deep learning

Yann Lecun
New York University
deep learning

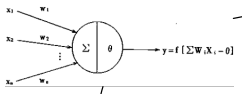
Capsule Nets(2017)

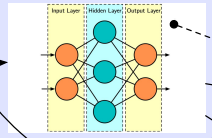


Kaiming He (何恺明)
MSRA => FAIR
computer vision

BPNN/MLP(1986)

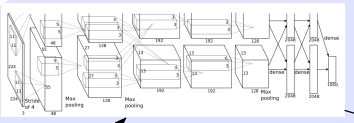
Perceptron(1958)

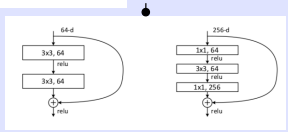




Neocognitron(1980)
[convolution & pooling]

AlexNet(2012)



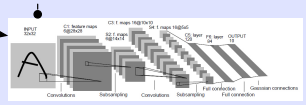


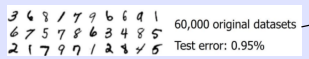
ResNet(2016)

VGG(2014)
GoogLeNet(2015)

DenseNet(2017)

LeNet/CNN(1998)

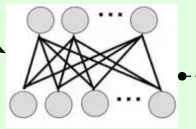




Relu, dropout & bigger

Hopfield Network(1982)
[recurrent & feedback]

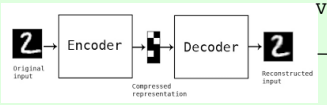
RBM(1986/2006)



stack

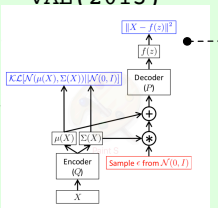
Deep Belief
Nets(2006)

AutoEncoder(1989/2006)
Denosing Autoencoder(2008)



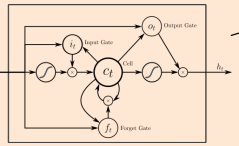
Variational
Inference

VAE(2013)



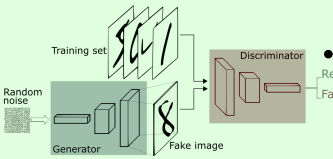
Max Welling
University of Amsterdam
statistical learning

RNN/LSTM(1997)



RNN in Speech
Recognition(2013)

GAN(2014)

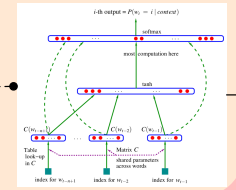


Ian Goodfellow
Google Brain
deep adversarial learning

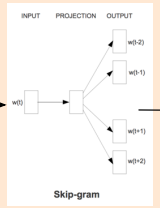
DCGAN(2014)
WGAN(2017)
PGGAN(2017)

SeqGAN(2017)
LeakGAN(2018)

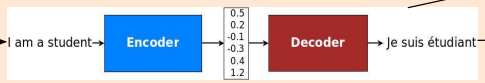
Neural Probabilistic
Language Model(2003)



word2Vec(2013)



Seq2Seq(2014)

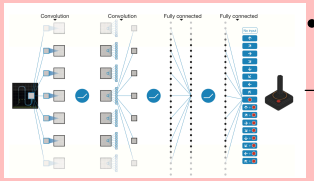


Character CNN(2015)
self-attention(2017)

Jürgen Schmidhuber
IDSIA
Universal AI

Yoshua Bengio
University of Montreal
Deep learning

Deep Q-
learning(2013)

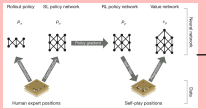


Double DQN(2015)
Dueling Net(2016)

David Silver
DeepMind
Reinforcement learning

DDPG(2015) → A3C(2016)

AlphaGo(2016)



Alpha Zero(2017)

Networked World

facebook

- 2 billion MAU
- 26.4 billion minutes/day

Alibaba Group 阿里巴巴集团

- >777 million trans. (alipay)
- 200 billion on 11/11

twitter

- 320 million MAU
- Peak: 143K tweets/s

新浪微博 weibo.com

- 462 million users
- influencing our daily life

Instagram

- 700 million MAU
- 95 million pics/day

头条 今日头条

- ~1.5 billion MAU
- 70 minutes/user/day

snapchat

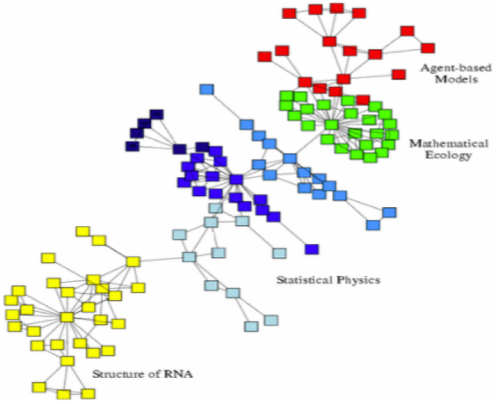
- 300 million MAU
- 30 minutes/user/day

WeChat

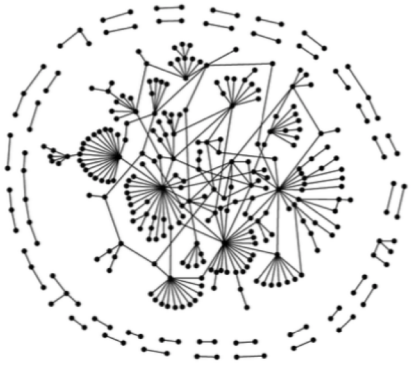
- QQ: 860 million MAU
- WeChat: 1.1 billion MAU

Many Data are Networks[1]

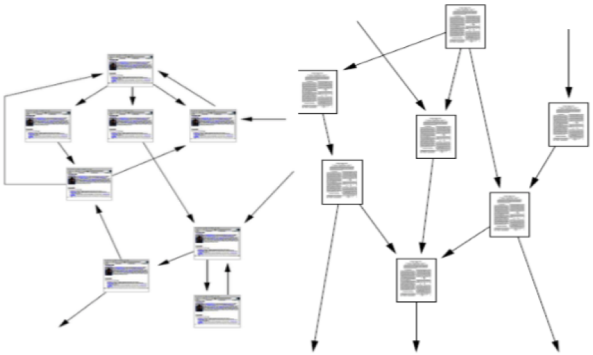
Social networks



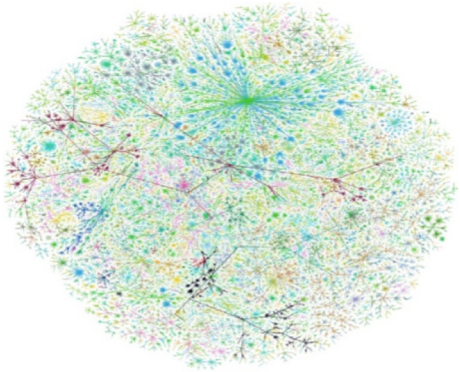
Economic networks



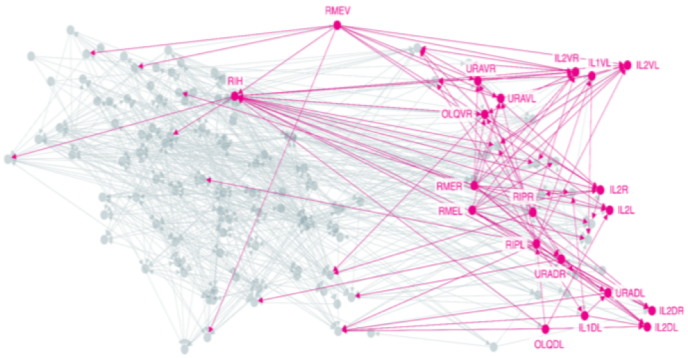
Biomedical networks



Information networks:
Web & citations



Internet



Networks of neurons

1. Example from Jure's slides

Machine Learning with Networks

- ML tasks in networks:
  - Node classification
    - Predict a type of a given node
  - Link prediction
    - Predict whether two nodes are linked
  - Community detection
    - Identify densely linked clusters of nodes
  - Network similarity
    - How similar are two (sub)networks?

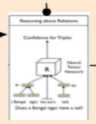
NE&GNN

Andrew Ng
Stanford University
Machine learning

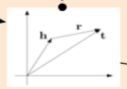
Antoine Bordes
Facebook
Deep learning

Distributed representation(1986)

Structured Embedding (2011)



neural tensor network(2013)



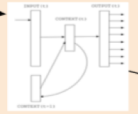
TransE(2013)

TransH(2014)
TransR(2015)
TransA(2015)
TransG(2016)

Yoshua Bengio
University of Montreal
Deep learning

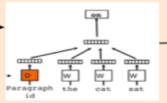
Geoffery Hinton
University of Toronto
Deep Learning

Neural Probabilistic Language Model(2003)



RNN based language model(2010)

word2Vec(2013)



Doc2vec(2014)

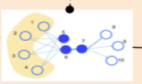
context2vec(2016)
ELMo(2018)
OpenAI GPT(2018)
BERT(2018)

Bryan Perozzi
Stony Brook University —>google
Data Mining

Tomas Mikolov
Google -> Facebook
NLP

Jian Tang
University of Montreal
Data Mining

Deepwalk (2014)



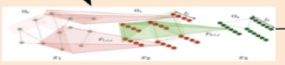
LINE (2015)

Node2vec(2016)

NetMF(2018)
NetSMF(2019)

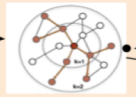
Graph Neural Networks (2005,2009)

Marco Gori
University of Siena
Machine Learning



Graph Covolutional Networks (2014)

GCN for semi-supervised classification (2017)



graphSAGE Inductive (2017)

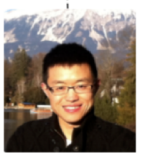
Graph Attention Network self-attention (2017)

Neural Message Passing(2017)

Yann Lecun
New York University
Deep Learning

Max Welling
University of Amsterdam
Statistical Learning

Jure Leskovec
Stanford University
Data Mining



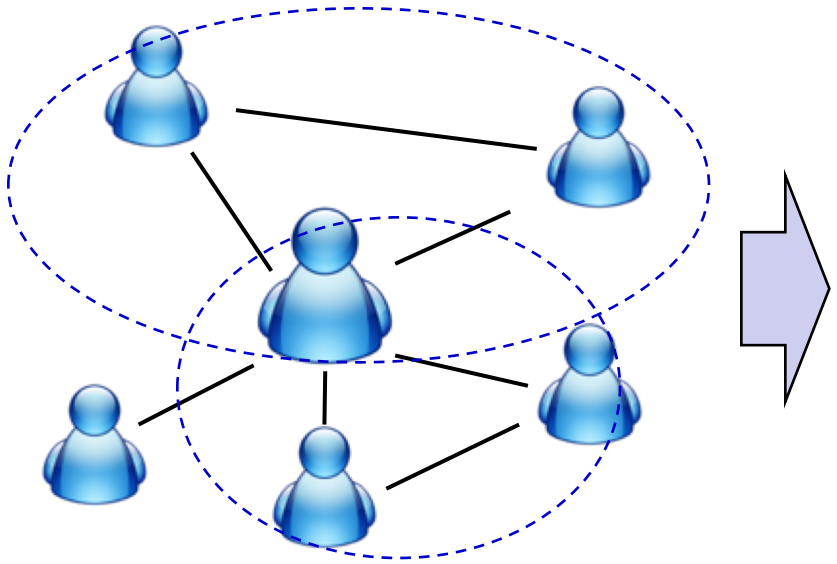
Jie Tang
Tsinghua University
Data Mining

回顾一下NE...

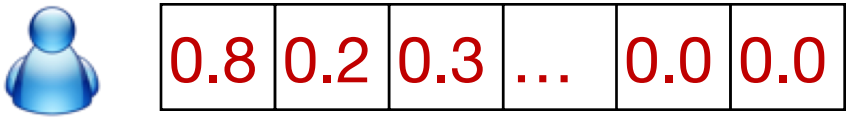
SEARCH

Review Representation Learning for Graphs

Representation Learning/
Graph Embedding

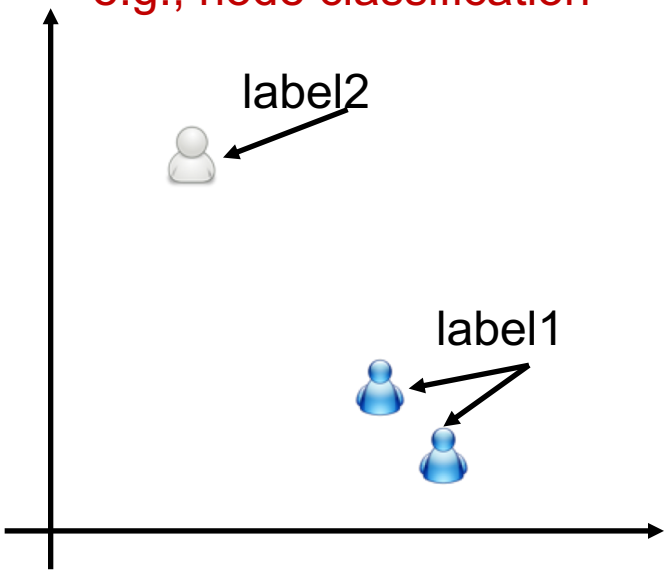


d-dimensional vector, $d << |V|$



Users with the same label are located in the *d*-dimensional space closer than those with different labels

e.g., node classification



Why is it hard?

- Modern deep learning toolbox is designed for simple sequences or grids.
  - CNNs for fixed-size images/grids...
  - RNNs or word2vec for text/sequences...
- But networks are far more complex!
  - Complex topographical structure (i.e., no spatial locality like grids)
  - No fixed node ordering or reference point (i.e., the isomorphism problem)
  - Often dynamic and have multimodal features.

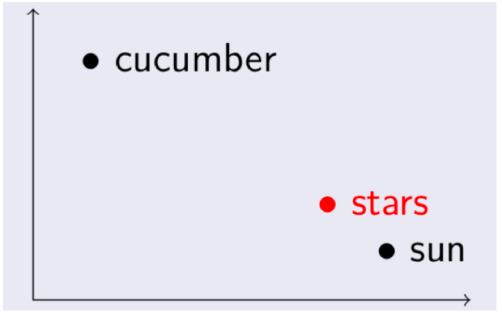
Recall word2vec for NLP

- Learning a representation for words:

$$\phi : v \in V \rightarrow R^d$$

```
he curtains open and the stars shining in on the barely
ars and the cold , close stars " . And neither of the w
rough the night with the stars shining so brightly , it
made in the light of the stars . It all boils down , wr
 surely under the bright stars , thrilled by ice-white
sun , the seasons of the stars ? Home , alone , Jay pla
m is dazzling snow , the stars have risen full and cold
```

	shining	bright	trees	dark	look
stars	38	45	2	27	12

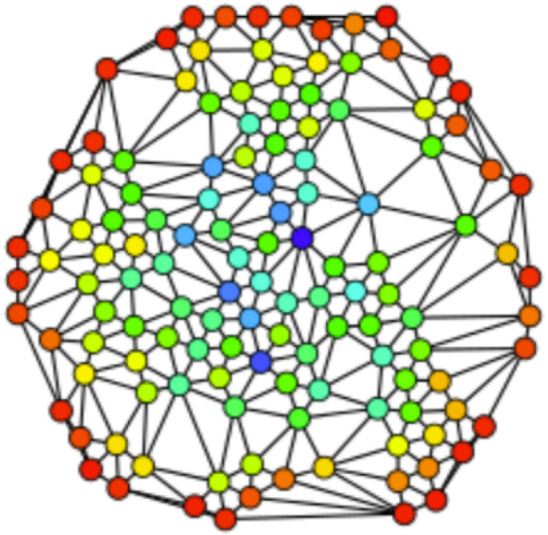


- Ideally, we should have

$$\|\phi(\text{sun}) - \phi(\text{stars})\| < \|\phi(\text{cucumber}) - \phi(\text{stars})\|$$

Node Embeddings

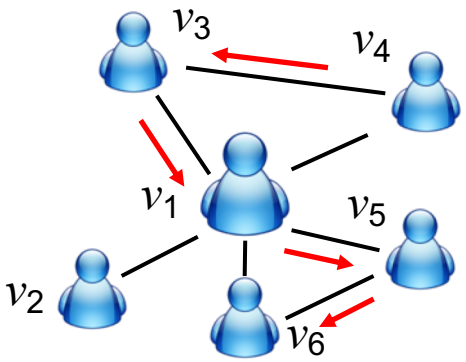
- How to learn a representation for each node of networks?



- Input: $G = (V, E)$ or adjacency matrix
- Problem decomposition:
  - how to generate the context for each vertex?
  - how to learn the representation effectively and efficiently?
  - how to incorporate the other unique network properties?
  - how to combine network and content together?

DeepWalk

Random walk



One example RW path

$v_4 \quad v_3 \quad v_1 \quad v_5 \quad v_6$

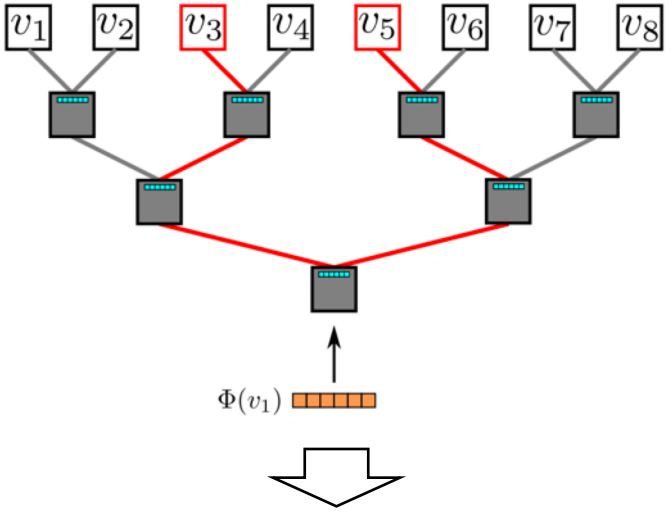
$\mathcal{W}_{v_4} = 4$

$u_k \begin{bmatrix} 3 \\ 1 \\ 5 \end{bmatrix} v_j \rightarrow$ Φ (d × j)

1

$\vdots$

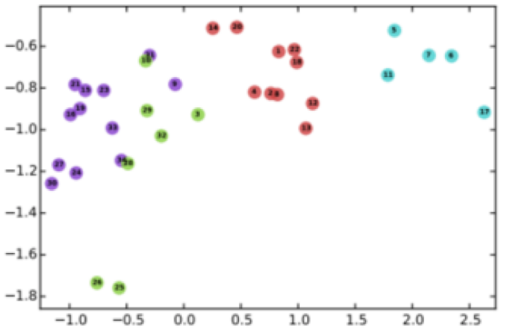
SkipGram with Hierarchical softmax



$$P(\{v_{i-w}, \cdots, v_{i+w}\} \backslash v_i | \Phi(v_i))) = \prod_{j=i-w, j \neq i}^{i+w} P(v_j | \Phi(v_i))$$

Hierarchical softmax

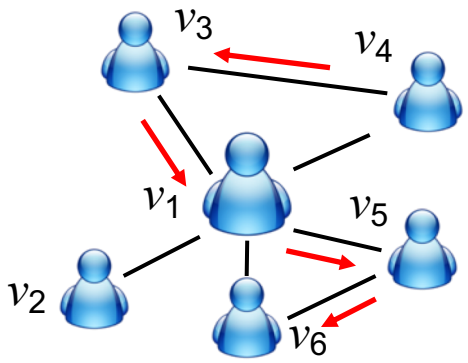
$$P(v_j | \Phi(v_i)) = \prod_{l=1}^{\log |V|} P(b_l | \Phi(v_i)) = \prod_{l=1}^{\log |V|} 1/(1 + e^{-\Phi(v_i) \cdot \Psi(b_l)})$$



1. B. Perozzi, R. Al-Rfou, and S. Skiena. 2014. Deepwalk: Online learning of social representations. *KDD*, 701–710.

DeepWalk

Random walk



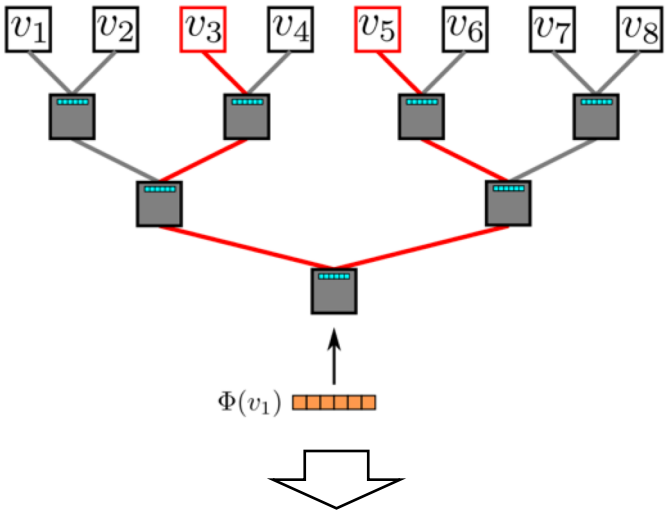
One example RW path

$v_4 \quad v_3 \quad v_1 \quad v_5 \quad v_6$

$\mathcal{W}_{v_4} = \begin{matrix} 4 \\ \begin{bmatrix} 3 \\ 1 \\ 5 \end{bmatrix} \\ 1 \\ \vdots \end{matrix}$

u_k v_j → Φ (d × j)

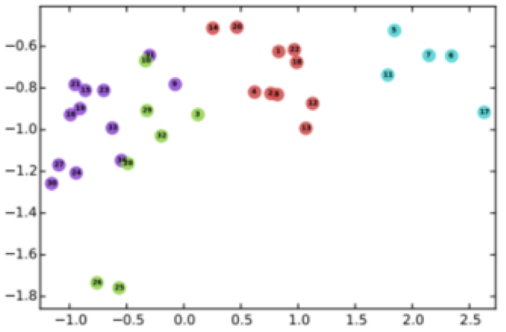
SkipGram with
Hierarchical softmax



$$P(\{v_{i-w}, \cdots, v_{i+w}\} \backslash v_i | \Phi(v_i))) = \prod_{j=i-w, j \neq i}^{i+w} P(v_j | \Phi(v_i))$$

Hierarchical softmax

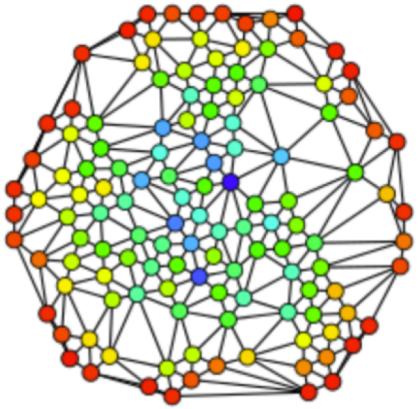
$$P(v_j | \Phi(v_i)) = \prod_{l=1}^{\log |V|} P(b_l | \Phi(v_i)) = \prod_{l=1}^{\log |V|} 1/(1 + e^{-\Phi(v_i) \cdot \Psi(b_l)})$$



1. B. Perozzi, R. Al-Rfou, and S. Skiena. 2014. Deepwalk: Online learning of social representations. *KDD*, 701–710.

Random Walk

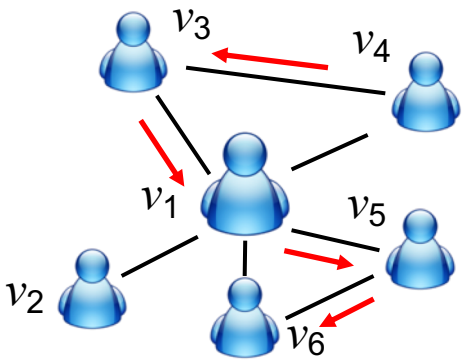
- Generate γ random walks for each vertex
- Each random walk has length t
  - in each random walk step, jump to the next vertex uniformly.
- Example: $v_{46} \rightarrow v_{45} \rightarrow v_{71} \rightarrow v_{24} \rightarrow v_5 \rightarrow v_1 \rightarrow v_{17}$
- Finally, for vertex v_1 in a network, we have



$$
\begin{array}{cccccc}
v_{71} \rightarrow & v_{24} \rightarrow & v_5 \rightarrow & v_1 \rightarrow & v_{17} \rightarrow & v_{80} \rightarrow \\
v_{92} \rightarrow & v_2 \rightarrow & v_3 \rightarrow & v_1 \rightarrow & v_{12} \rightarrow & v_{73} \rightarrow \\
v_{37} \rightarrow & v_{34} \rightarrow & v_9 \rightarrow & v_1 \rightarrow & v_{10} \rightarrow & v_{94} \rightarrow \\
v_{73} \rightarrow & v_{64} \rightarrow & v_5 \rightarrow & v_1 \rightarrow & v_{12} \rightarrow & v_1 \rightarrow \\
v_{75} \rightarrow & v_{14} \rightarrow & v_6 \rightarrow & v_1 \rightarrow & v_{13} \rightarrow & v_{61} \rightarrow
\end{array}
$$

DeepWalk

Random walk



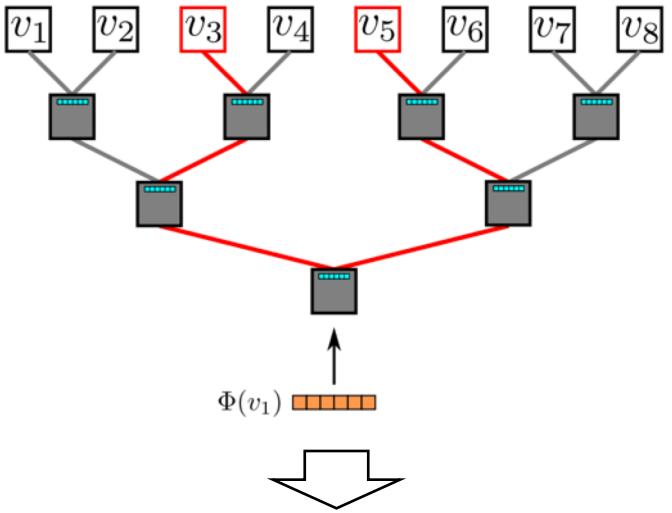
One example RW path

$v_4 \quad v_3 \quad v_1 \quad v_5 \quad v_6$

$\mathcal{W}_{v_4} = 4$

$u_k \begin{bmatrix} 3 \\ 1 \\ 5 \\ 1 \\ \vdots \end{bmatrix} v_j \rightarrow$ Φ (d × j)

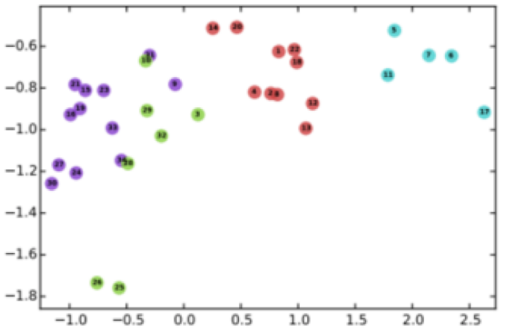
SkipGram with Hierarchical softmax



$$P(\{v_{i-w}, \cdots, v_{i+w}\} \backslash v_i | \Phi(v_i))) = \prod_{j=i-w, j \neq i}^{i+w} P(v_j | \Phi(v_i))$$

Hierarchical softmax

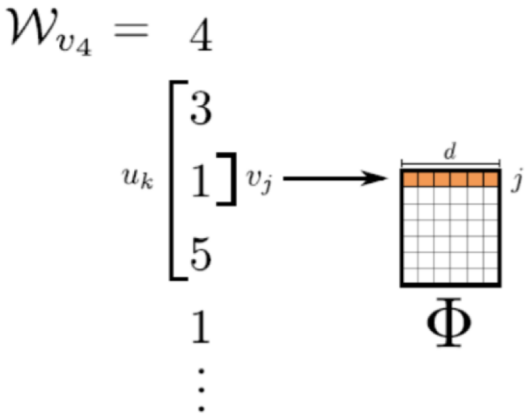
$$P(v_j | \Phi(v_i)) = \prod_{l=1}^{\log |V|} P(b_l | \Phi(v_i)) = \prod_{l=1}^{\log |V|} 1/(1 + e^{-\Phi(v_i) \cdot \Psi(b_l)})$$



1. B. Perozzi, R. Al-Rfou, and S. Skiena. 2014. Deepwalk: Online learning of social representations. *KDD*, 701–710.

Representation Mapping

- For a path $\mathcal{W}_{v_4}$: $v_4 \rightarrow v_3 \rightarrow v_1 \rightarrow v_5 \rightarrow v_1 \rightarrow v_{46}$

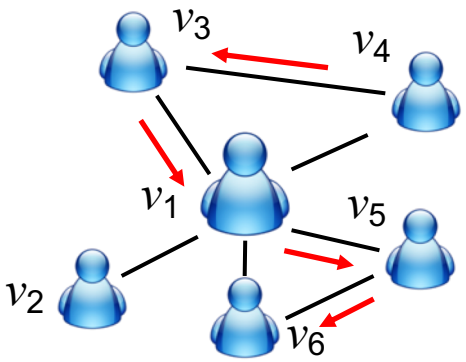


- Define a window size **w**: if $\mathbf{w} = 1$ then $\mathbf{v} = v_1$
- Map the current vertex v_1 to its representation in R^d
- Maximize (skip-gram)

$$P(v_3, v_5 | \phi(v_1))$$

DeepWalk

Random walk



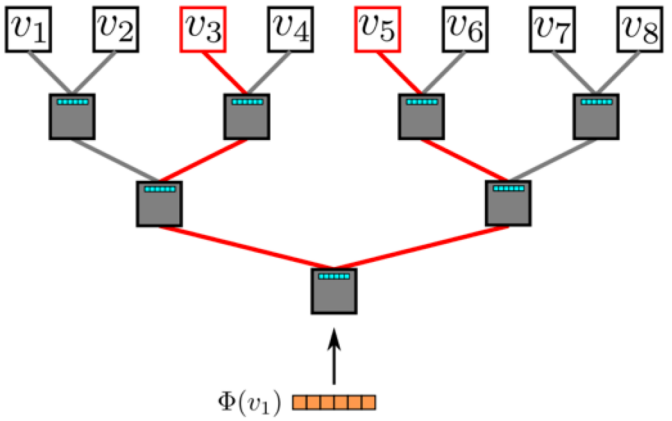
One example RW path

$v_4 \quad v_3 \quad v_1 \quad v_5 \quad v_6$

$\mathcal{W}_{v_4} = \begin{bmatrix} 4 \\ 3 \\ 1 \\ 5 \\ 1 \\ \vdots \end{bmatrix}$

u_k v_j → Φ (d × j)

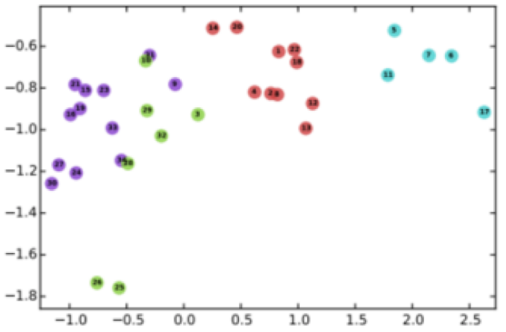
SkipGram with Hierarchical softmax



$$P(\{v_{i-w}, \cdots, v_{i+w}\} \backslash v_i | \Phi(v_i))) = \prod_{j=i-w, j \neq i}^{i+w} P(v_j | \Phi(v_i))$$

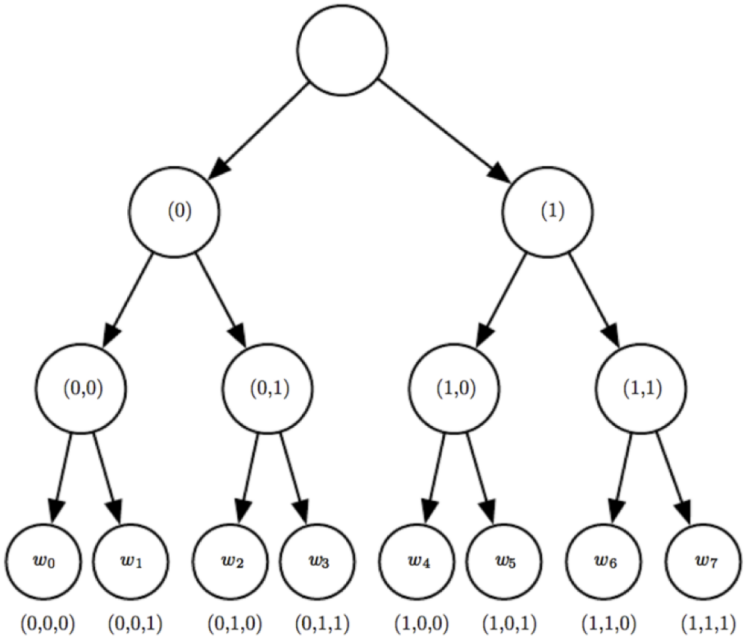
Hierarchical softmax

$$P(v_j | \Phi(v_i)) = \prod_{l=1}^{\log |V|} P(b_l | \Phi(v_i)) = \prod_{l=1}^{\log |V|} 1/(1 + e^{-\Phi(v_i) \cdot \Psi(b_l)})$$



1. B. Perozzi, R. Al-Rfou, and S. Skiena. 2014. Deepwalk: Online learning of social representations. *KDD*, 701–710.

Hierarchical Softmax



- Then

$$p(v_i|C_i) = \prod_{k=1}^{K} p(d_k|q_k, C_i) = \prod_{k=1}^{K} \left(\sigma(q_k \cdot C_i)^{1-d_k} (1 - \sigma(q_k \cdot C_i))^{d_k} \right)$$

where σ is the sigmoid function, q_k is the vector of non-leaf node on the path from root to word leaf, d_k is the corresponding code of q_k.

Parameter Learning

- Randomly initialize the representations
- Each classifier in the hierarchy has a set of weights
- Use SGD (stochastic gradient descent) to update both classifier weights and vertex representations simultaneously

Results: BlogCatalog

Name	BlogCatalog
$\|V\|$	10,312
$\|E\|$	333,983
$\|\mathcal{Y}\|$	39
Labels	Interests

	% Labeled Nodes	10%	20%	30%	40%	50%	60%	70%	80%	90%
Micro-F1(%)	DeepWalk	**36.00**	**38.20**	**39.60**	**40.30**	**41.00**	**41.30**	41.50	41.50	42.00
	SpectralClustering	31.06	34.95	37.27	38.93	39.97	40.99	**41.66**	**42.42**	**42.62**
	EdgeCluster	27.94	30.76	31.85	32.99	34.12	35.00	34.63	35.99	36.29
	Modularity	27.35	30.74	31.77	32.97	34.09	36.13	36.08	37.23	38.18
	wvRN	19.51	24.34	25.62	28.82	30.37	31.81	32.19	33.33	34.28
	Majority	16.51	16.66	16.61	16.70	16.91	16.99	16.92	16.49	17.26
Macro-F1(%)	DeepWalk	**21.30**	**23.80**	25.30	26.30	27.30	27.60	27.90	28.20	28.90
	SpectralClustering	19.14	23.57	**25.97**	**27.46**	**28.31**	**29.46**	**30.13**	**31.38**	**31.78**
	EdgeCluster	16.16	19.16	20.48	22.00	23.00	23.64	23.82	24.61	24.92
	Modularity	17.36	20.00	20.80	21.85	22.65	23.41	23.89	24.20	24.97
	wvRN	6.25	10.13	11.64	14.24	15.86	17.18	17.98	18.86	19.57
	Majority	2.52	2.55	2.52	2.58	2.58	2.63	2.61	2.48	2.62

- Feed the learned representation for multi-label classification
- DeepWalk (vertex representation learning) performs well, especially when labels are sparse.

Results: YouTube

Name	YouTube
$\|V\|$	1,138,499
$\|E\|$	2,990,443
$\|\mathcal{Y}\|$	47
Labels	Groups

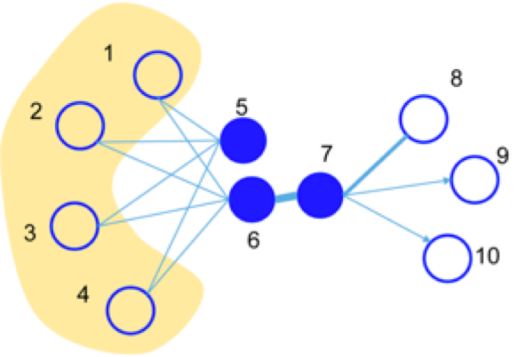
	% Labeled Nodes	1%	2%	3%	4%	5%	6%	7%	8%	9%	10%
Micro-F1(%)	DeepWalk	**37.95**	**39.28**	**40.08**	**40.78**	**41.32**	**41.72**	**42.12**	**42.48**	**42.78**	**43.05**
	SpectralClustering	—	—	—	—	—	—	—	—	—	—
	EdgeCluster	23.90	31.68	35.53	36.76	37.81	38.63	38.94	39.46	39.92	40.07
	Modularity	—	—	—	—	—	—	—	—	—	—
	wvRN	26.79	29.18	33.1	32.88	35.76	37.38	38.21	37.75	38.68	39.42
	Majority	24.90	24.84	25.25	25.23	25.22	25.33	25.31	25.34	25.38	25.38
Macro-F1(%)	DeepWalk	**29.22**	**31.83**	**33.06**	**33.90**	**34.35**	**34.66**	**34.96**	**35.22**	**35.42**	**35.67**
	SpectralClustering	—	—	—	—	—	—	—	—	—	—
	EdgeCluster	19.48	25.01	28.15	29.17	29.82	30.65	30.75	31.23	31.45	31.54
	Modularity	—	—	—	—	—	—	—	—	—	—
	wvRN	13.15	15.78	19.66	20.9	23.31	25.43	27.08	26.48	28.33	28.89
	Majority	6.12	5.86	6.21	6.1	6.07	6.19	6.17	6.16	6.18	6.19

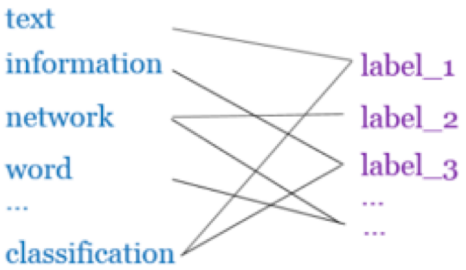
- Similar results on YouTube
- Spectral Clustering does not scale to large graphs

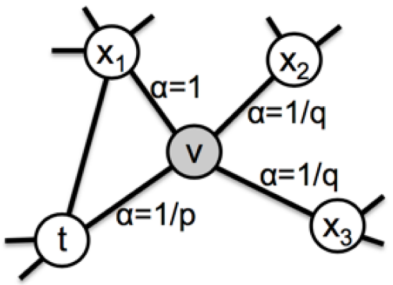
- DeepWalk utilizes fixed-length, unbiased random walks to generate context for each node, can we do better?

Later…

- LINE[1]: explicitly preserves both *first-order* and *second-order* proximities.
- PTE[2]: learn heterogeneous text network embedding via a semi-supervised manner.
- Node2vec[3]: use a biased random walk to better explore node's neighborhood.







1. J. Tang, M. Qu, M. Wang, M. Zhang, J. Yan, and Q. Mei. 2015. Line: Large-scale information network embedding. *WWW*, 1067–1077.
2. J. Tang, M. Qu, and Q. Mei. 2015. Pte: Predictive text embedding through large-scale heterogeneous text networks. *KDD*, 1165–1174.
3. A. Grover and J. Leskovec. 2016. node2vec: Scalable feature learning for networks. *KDD*, 855–864.

Questions

- What are the fundamentals underlying the different models?

or

- Can we unify the different graph embedding approaches?

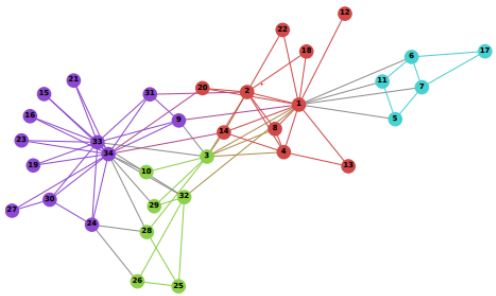
Unifying DeepWalk, LINE, PTE, and node2vec into Matrix Forms

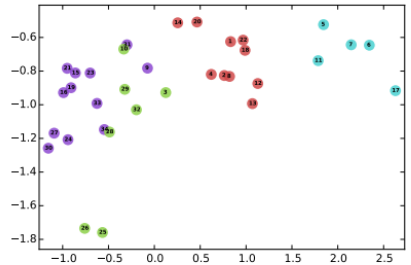
Algorithm	Closed Matrix Form
DeepWalk	$\log\left(\mathrm{vol}(G)\left(\frac{1}{T}\sum_{r=1}^{T}(\boldsymbol{D}^{-1}\boldsymbol{A})^r\right)\boldsymbol{D}^{-1}\right)-\log b$
LINE	$\log\left(\mathrm{vol}(G)\boldsymbol{D}^{-1}\boldsymbol{A}\boldsymbol{D}^{-1}\right)-\log b$
PTE	$\log\left(\begin{bmatrix}\alpha\,\mathrm{vol}(G_{\mathrm{ww}})(\boldsymbol{D}^{\mathrm{ww}}_{\mathrm{row}})^{-1}\boldsymbol{A}_{\mathrm{ww}}(\boldsymbol{D}^{\mathrm{ww}}_{\mathrm{col}})^{-1}\\ \beta\,\mathrm{vol}(G_{\mathrm{dw}})(\boldsymbol{D}^{\mathrm{dw}}_{\mathrm{row}})^{-1}\boldsymbol{A}_{\mathrm{dw}}(\boldsymbol{D}^{\mathrm{dw}}_{\mathrm{col}})^{-1}\\ \gamma\,\mathrm{vol}(G_{\mathrm{lw}})(\boldsymbol{D}^{\mathrm{lw}}_{\mathrm{row}})^{-1}\boldsymbol{A}_{\mathrm{lw}}(\boldsymbol{D}^{\mathrm{lw}}_{\mathrm{col}})^{-1}\end{bmatrix}\right)-\log b$
node2vec	$\log\left(\frac{\frac{1}{2T}\sum_{r=1}^{T}\left(\sum_u \boldsymbol{X}_{w,u}\underline{\boldsymbol{P}}^r_{c,w,u}+\sum_u \boldsymbol{X}_{c,u}\underline{\boldsymbol{P}}^r_{w,c,u}\right)}{\left(\sum_u \boldsymbol{X}_{w,u}\right)\left(\sum_u \boldsymbol{X}_{c,u}\right)}\right)-\log b$

$\boldsymbol{A}$: $\boldsymbol{A}\in\mathbb{R}_{+}^{|V|\times|V|}$ is G's adjacency matrix with $\boldsymbol{A}_{i,j}$ as the edge weight between vertices i and j;
$\boldsymbol{D}_{\mathrm{col}}$: $\boldsymbol{D}_{\mathrm{col}}=\mathrm{diag}(\boldsymbol{A}^{\top}\boldsymbol{e})$ is the diagonal matrix with column sum of $\boldsymbol{A}$;
$\boldsymbol{D}_{\mathrm{row}}$: $\boldsymbol{D}_{\mathrm{row}}=\mathrm{diag}(\boldsymbol{A}\boldsymbol{e})$ is the diagonal matrix with row sum of $\boldsymbol{A}$;
$\boldsymbol{D}$: For undirected graphs ($\boldsymbol{A}^{\top}=\boldsymbol{A}$), $\boldsymbol{D}_{\mathrm{col}}=\boldsymbol{D}_{\mathrm{row}}$. For brevity, $\boldsymbol{D}$ represents both $\boldsymbol{D}_{\mathrm{col}}$ & $\boldsymbol{D}_{\mathrm{row}}$.
$\boldsymbol{D}=\mathrm{diag}(d_1,\cdots,d_{|V|})$, where d_i represents generalized degree of vertex i;
$\mathrm{vol}(G)$: $\mathrm{vol}(G)=\sum_i\sum_j \boldsymbol{A}_{i,j}=\sum_i d_i$ is the volume of an weighted graph G;
T & b: The context window size and the number of negative sampling in skip-gram, respectively.

1. Qiu et al. Network embedding as matrix factorization: unifying deepwalk, line, pte, and node2vec. *WSDM'18.* **The most cited paper in WSDM'18 as of May 2019**

DeepWalk is factorizing a matrix





DeepWalk is asymptotically and implicitly factorizing

$$\log\left(\frac{\mathrm{vol}(G)}{b}\left(\frac{1}{T}\sum_{r=1}^{T}\left(\boldsymbol{D}^{-1}\boldsymbol{A}\right)^{r}\right)\boldsymbol{D}^{-1}\right)$$

$$vol(G) = \sum_i \sum_j A_{ij}$$

$\boldsymbol{A}$ Adjacency matrix

$\boldsymbol{D}$ Degree matrix

b: #negative samples

T: context window size

LINE

- Objective of LINE:

$$\mathcal{L} = \sum_{i=1}^{|V|} \sum_{j=1}^{|V|} \left(\boldsymbol{A}_{i,j} \log g\left(\boldsymbol{x}_i^\top \boldsymbol{y}_j\right) + \frac{b d_i d_j}{\mathrm{vol}(G)} \log g\left(-\boldsymbol{x}_i^\top \boldsymbol{y}_j\right) \right).$$

- Align it with the Objective of SGNS:

$$\mathcal{L} = \sum_{w} \sum_{c} \left(\#(w,c) \log g\left(\boldsymbol{x}_w^\top \boldsymbol{y}_c\right) + \frac{b \#(w) \#(c)}{|\mathcal{D}|} \log g\left(-\boldsymbol{x}_w^\top \boldsymbol{y}_c\right) \right).$$

- LINE is actually factorizing

$$\log \left(\frac{\mathrm{vol}(G)}{b} \boldsymbol{D}^{-1} \boldsymbol{A} \boldsymbol{D}^{-1} \right)$$

- Recall DeepWalk's matrix form:

$$\log \left(\frac{\mathrm{vol}(G)}{b} \left(\frac{1}{T} \sum_{r=1}^{T} \left(\boldsymbol{D}^{-1} \boldsymbol{A} \right)^r \right) \boldsymbol{D}^{-1} \right).$$

Observation LINE is a special case of DeepWalk ($T = 1$).

PTE

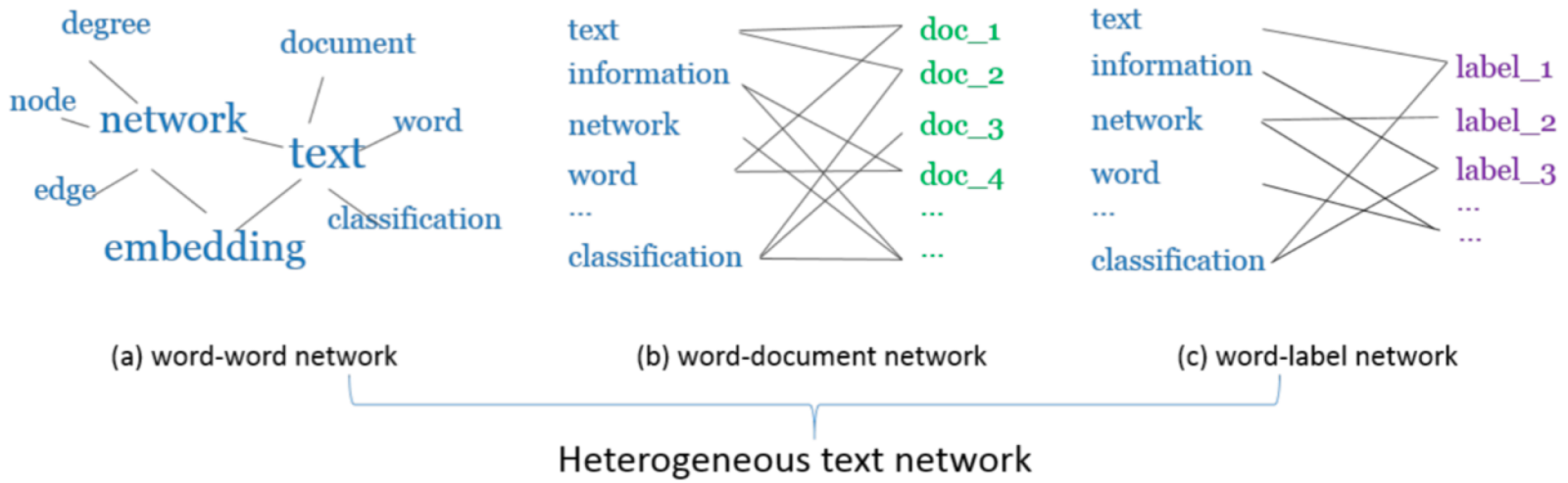
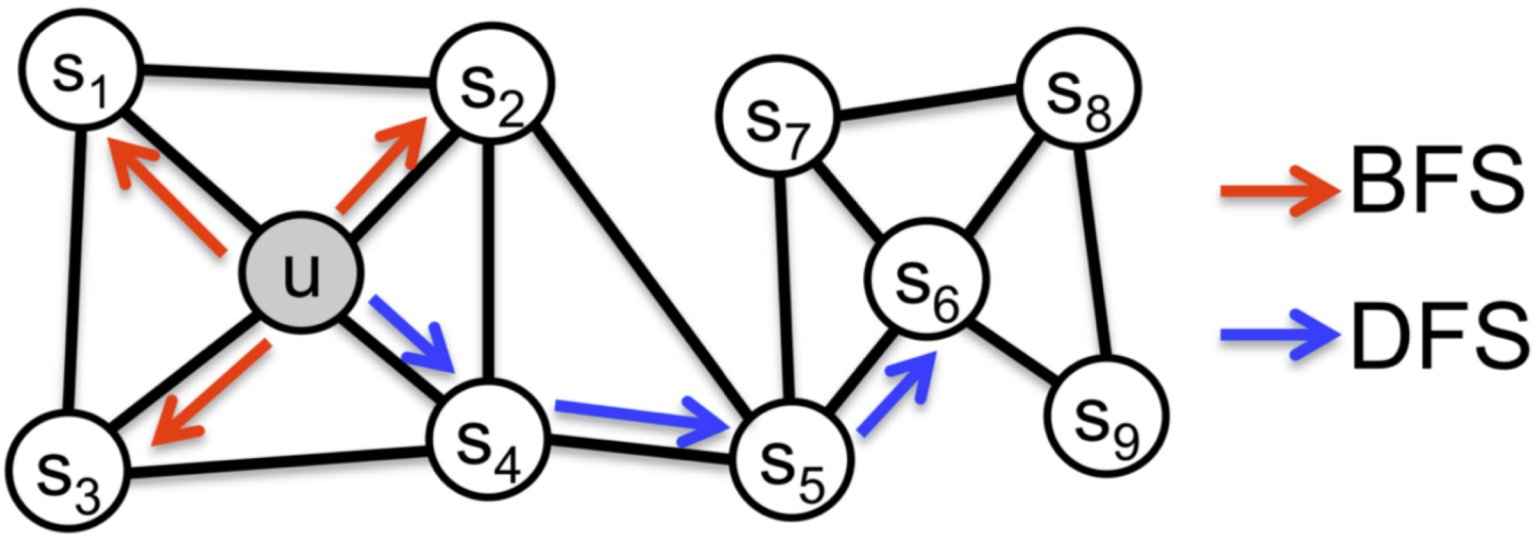


Figure 2: Heterogeneous Text Network.

$$\log\left(\begin{bmatrix}\alpha\,\mathrm{vol}(G_{\mathsf{ww}})(\boldsymbol{D}_{\mathsf{row}}^{\mathsf{ww}})^{-1}\boldsymbol{A}_{\mathsf{ww}}(\boldsymbol{D}_{\mathsf{col}}^{\mathsf{ww}})^{-1}\\ \beta\,\mathrm{vol}(G_{\mathsf{dw}})(\boldsymbol{D}_{\mathsf{row}}^{\mathsf{dw}})^{-1}\boldsymbol{A}_{\mathsf{dw}}(\boldsymbol{D}_{\mathsf{col}}^{\mathsf{dw}})^{-1}\\ \gamma\,\mathrm{vol}(G_{\mathsf{lw}})(\boldsymbol{D}_{\mathsf{row}}^{\mathsf{lw}})^{-1}\boldsymbol{A}_{\mathsf{lw}}(\boldsymbol{D}_{\mathsf{col}}^{\mathsf{lw}})^{-1}\end{bmatrix}\right)-\log b,$$

node2vec: Biased Walks

- Use biased random walks to trade off local and global views of the network



- Biased walks is a special case of random walk, thus node2vec is a special case of DeepWalk

1. A. Grover and J. Leskovec. 2016. node2vec: Scalable feature learning for networks. *KDD*, 855–864.

Unifying DeepWalk, LINE, PTE, and node2vec into Matrix Forms

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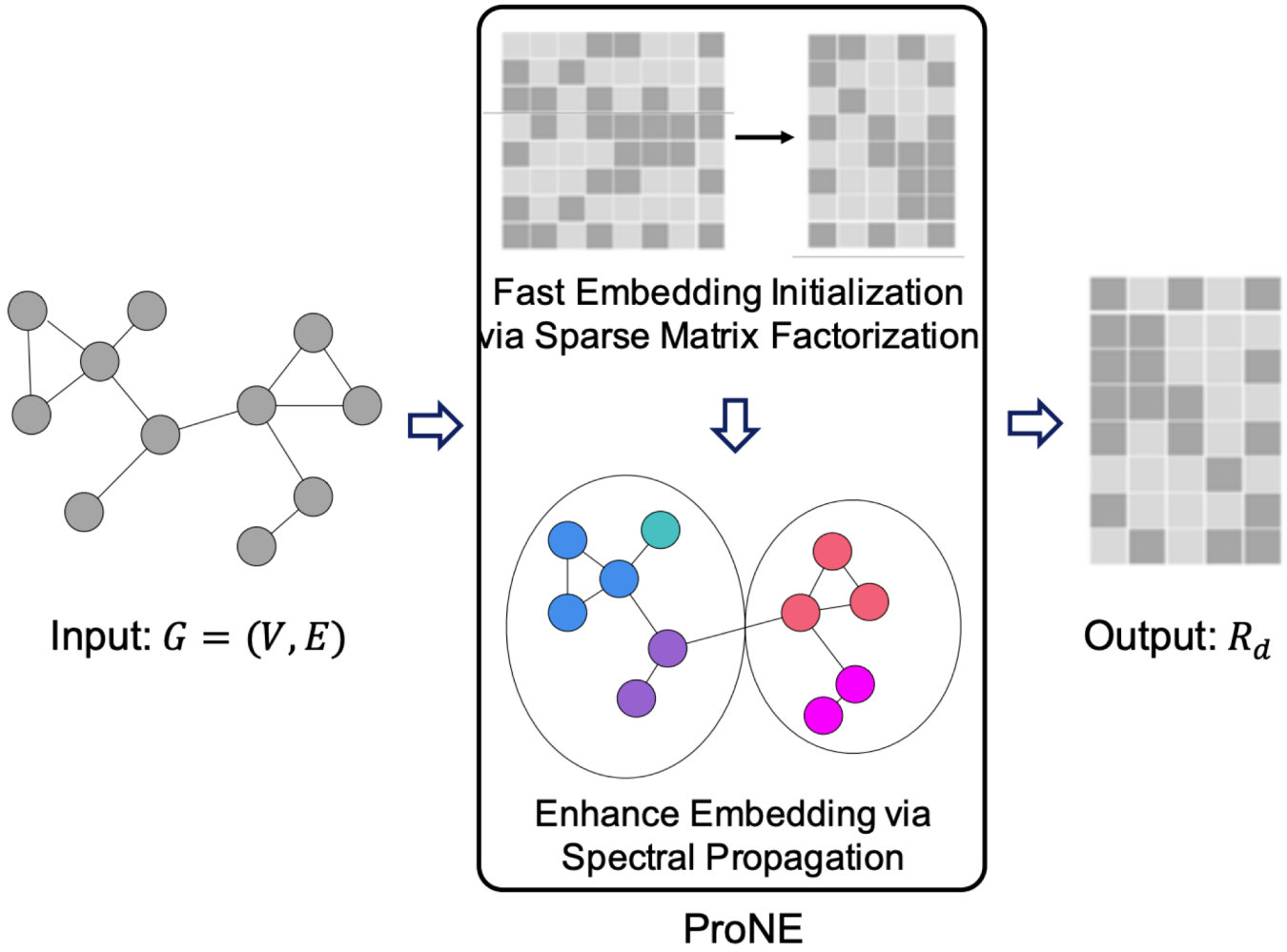
LINE	$\log\left(\mathrm{vol}(G)\boldsymbol{D}^{-1}\boldsymbol{A}\boldsymbol{D}^{-1}\right)-\log b$
PTE	$\log\left(\begin{bmatrix}\alpha\,\mathrm{vol}(G_{\mathrm{ww}})(\boldsymbol{D}_{\mathrm{row}}^{\mathrm{ww}})^{-1}\boldsymbol{A}_{\mathrm{ww}}(\boldsymbol{D}_{\mathrm{col}}^{\mathrm{ww}})^{-1}\\ \beta\,\mathrm{vol}(G_{\mathrm{dw}})(\boldsymbol{D}_{\mathrm{row}}^{\mathrm{dw}})^{-1}\boldsymbol{A}_{\mathrm{dw}}(\boldsymbol{D}_{\mathrm{col}}^{\mathrm{dw}})^{-1}\\ \gamma\,\mathrm{vol}(G_{\mathrm{lw}})(\boldsymbol{D}_{\mathrm{row}}^{\mathrm{lw}})^{-1}\boldsymbol{A}_{\mathrm{lw}}(\boldsymbol{D}_{\mathrm{col}}^{\mathrm{lw}})^{-1}\end{bmatrix}\right)-\log b$
node2vec	$\log\left(\frac{\frac{1}{2T}\sum_{r=1}^{T}\left(\sum_u \boldsymbol{X}_{w,u}\underline{\boldsymbol{P}}_{c,w,u}^{r}+\sum_u \boldsymbol{X}_{c,u}\underline{\boldsymbol{P}}_{w,c,u}^{r}\right)}{\left(\sum_u \boldsymbol{X}_{w,u}\right)\left(\sum_u \boldsymbol{X}_{c,u}\right)}\right)-\log b$

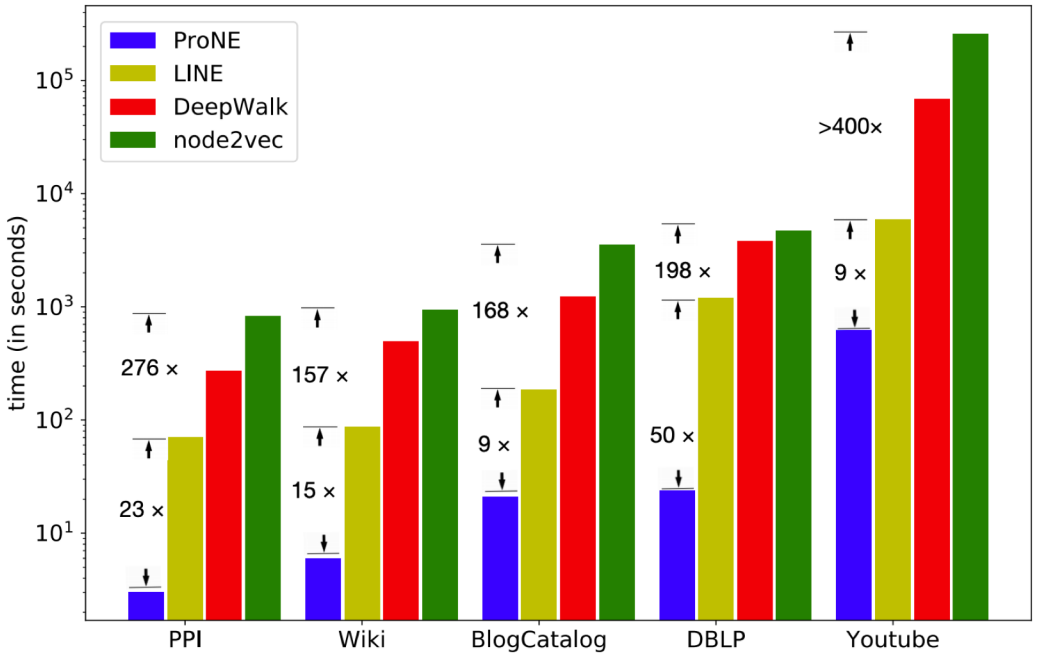
1. Qiu et al. Network embedding as matrix factorization: unifying deepwalk, line, pte, and node2vec. *WSDM'18.* **The most cited paper in WSDM'18 as of May 2019**

ProNE: Fast and Scalable Network Embedding



1. J. Zhang, Y. Dong, Y. Wang, J. Tang, and M. Ding. ProNE: Fast and Scalable Network Representation Learning. IJCAI'19.

Results



* ProNE (1 thread) v.s. Others (20 threads)

* 10 minutes on Youtube (~1M nodes)

Dataset	*DeepWalk*	*LINE*	*node2vec*	*ProNE*
PPI	272	70	828	**3**
Wiki	494	87	939	**6**
BlogCatalog	1,231	185	3,533	**21**
DBLP	3,825	1,204	4,749	**24**
Youtube	68,272	5,890	>5days	**627**

** Code available at https://github.com/THUDM/ProNE

Effectiveness experiments

Dataset	training ratio	0.1	0.3	0.5	0.7	0.9
PPI	DeepWalk	16.4	19.4	21.1	22.3	22.7
	LINE	16.3	20.1	21.5	22.7	23.1
	node2vec	16.2	19.7	21.6	23.1	24.1
	GraRep	15.4	18.9	20.2	20.4	20.9
	HOPE	16.4	19.8	21.0	21.7	22.5
	ProNE (SMF)	15.8	20.6	22.7	23.7	24.2
	ProNE	**18.2**	**22.7**	**24.6**	**25.4**	**25.9**
	($\pm\sigma$)	($\pm$0.5)	($\pm$0.3)	($\pm$0.7)	($\pm$1.0)	($\pm$1.1)
Wiki	DeepWalk	40.4	45.9	48.5	49.1	49.4
	LINE	**47.8**	50.4	51.2	51.6	52.4
	node2vec	45.6	47.0	48.2	49.6	50.0
	GraRep	47.2	49.7	50.6	50.9	51.8
	HOPE	38.5	39.8	40.1	40.1	40.1
	ProNE (SMF)	47.6	51.6	53.2	53.5	53.9
	ProNE	47.3	**53.1**	**54.7**	**55.2**	**57.2**
	($\pm\sigma$)	($\pm$0.7)	($\pm$0.4)	($\pm$0.8)	($\pm$0.8)	($\pm$1.3)
BlogCatalog	DeepWalk	36.2	39.6	40.9	41.4	42.2
	LINE	28.2	30.6	33.2	35.5	36.8
	node2vec	**36.3**	39.7	41.1	42.0	42.1
	GraRep	34.0	32.5	33.3	33.7	34.1
	Pro					

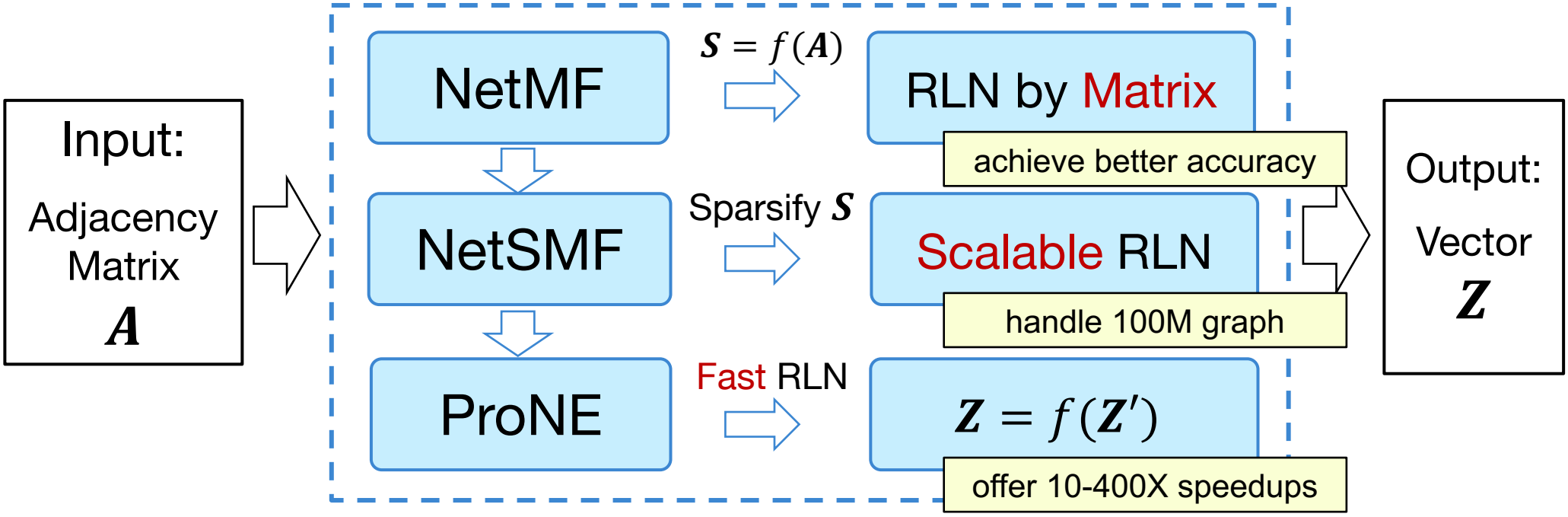
Dataset	training ratio	0.01	0.03	0.05	0.07	0.09
DBLP	DeepWalk	49.3	55.0	57.1	57.9	58.4
	LINE	48.7	52.6	53.5	54.1	54.5
	node2vec	48.9	55.1	57.0	58.0	58.4
	GraRep	50.5	52.6	53.2	53.5	53.8
	HOPE	**52.2**	55.0	55.9	56.3	56.6
	ProNE (SMF)	50.8	54.9	56.1	56.7	57.0
	ProNE	48.8	**56.2**	**58.0**	**58.8**	**59.2**
	($\pm\sigma$)	($\pm$1.0)	($\pm$0.5)	($\pm$0.2)	($\pm$0.2)	($\pm$0.1)
Youtube	DeepWalk	38.0	40.1	41.3	42.1	42.8
	LINE	33.2	35.5	37.0	38.2	39.3
	ProNE (SMF)	36.5	40.2	41.2	41.7	42.1
	ProNE	**38.2**	**41.4**	**42.3**	**42.9**	**43.3**
	($\pm\sigma$)	($\pm$0.8)	($\pm$0.3)	($\pm$0.2)	($\pm$0.2)	($\pm$0.2)

* ProNE (SMF) = ProNE w/ only sparse matrix factorization

Embed 100,000,000 nodes by one thread:
29 hours with **performance superiority**

** Code available at https://github.com/THUDM/ProNE

Representation Learning on Networks

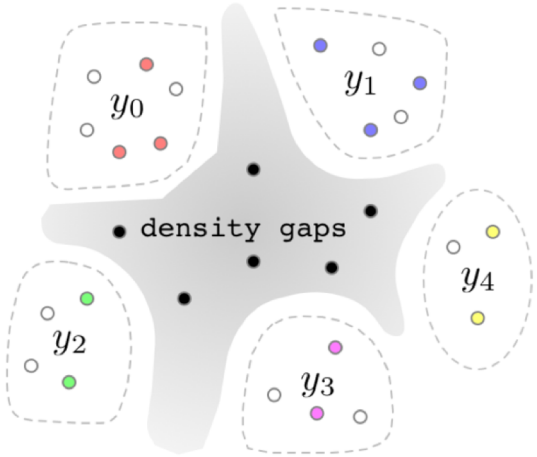


1. Qiu et al. Network embedding as matrix factorization: unifying deepwalk, line, pte, and node2vec. *WSDM'18.* **The most cited paper in WSDM'18 as of May 2019**
2. J. Qiu, Y. Dong, H. Ma, J. Li, C. Wang, K. Wang, and J. Tang. NetSMF: Large-Scale Network Embedding as Sparse Matrix Factorization. WWW'19.
3. J. Zhang, Y. Dong, Y. Wang, J. Tang, and M. Ding. ProNE: Fast and Scalable Network Representation Learning. IJCAI'19.

GNN时代...

SEARCH

Recent GCN Research



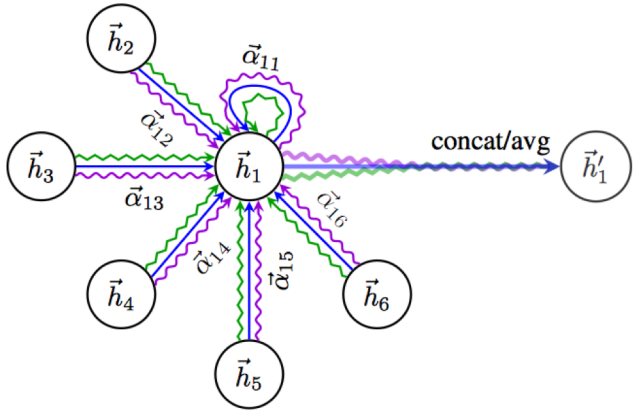
2018 GraphSGAN

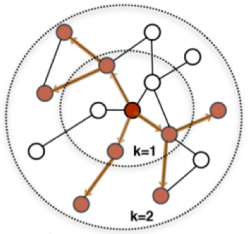
FastGCN 2018

2018 GAT

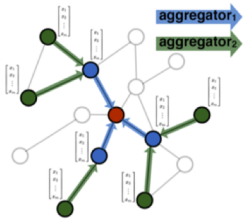
GraphSAGE 2017

2017 GCN

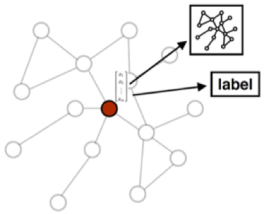




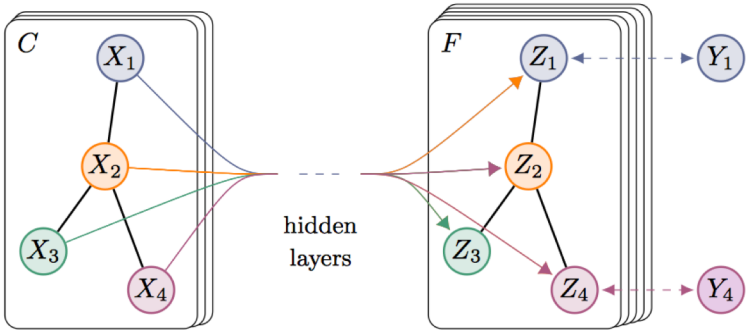
1. Sample neighborhood



2. Aggregate feature information from neighbors

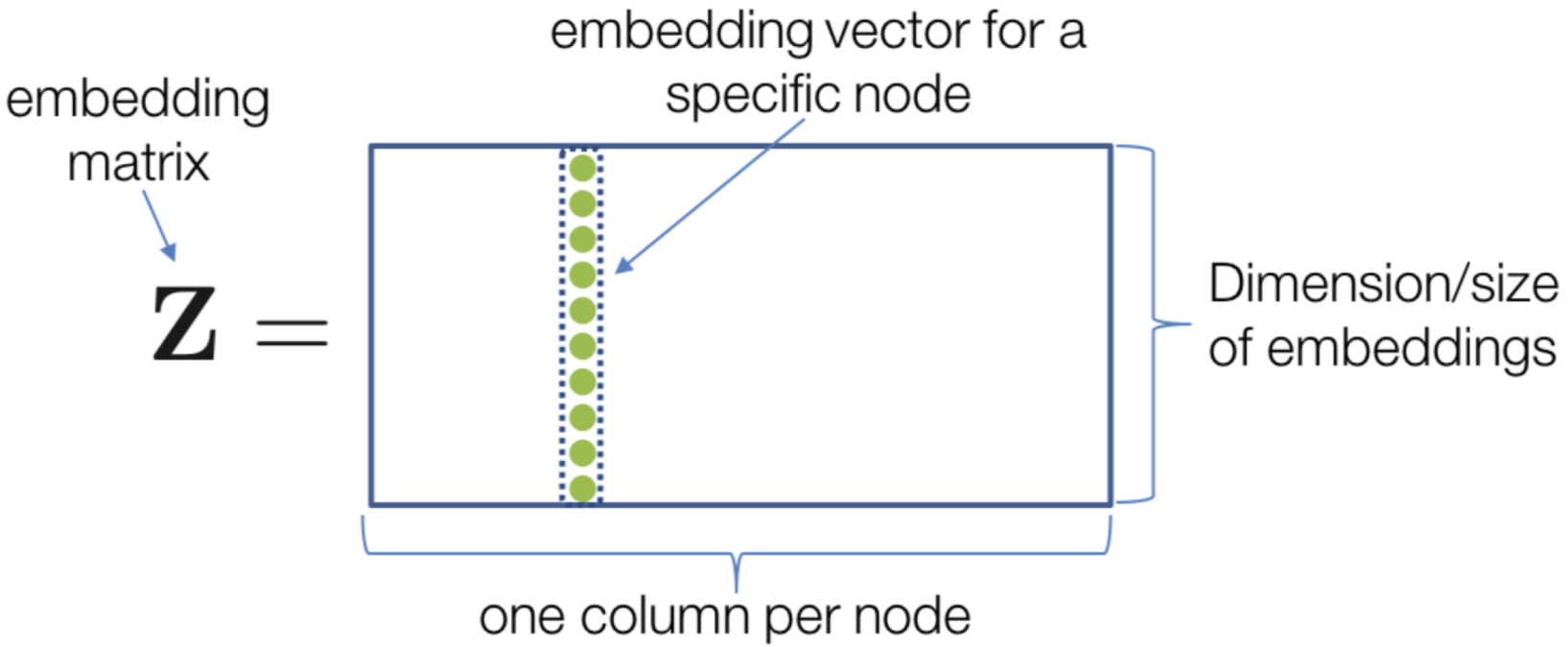


3. Predict graph context and label using aggregated information



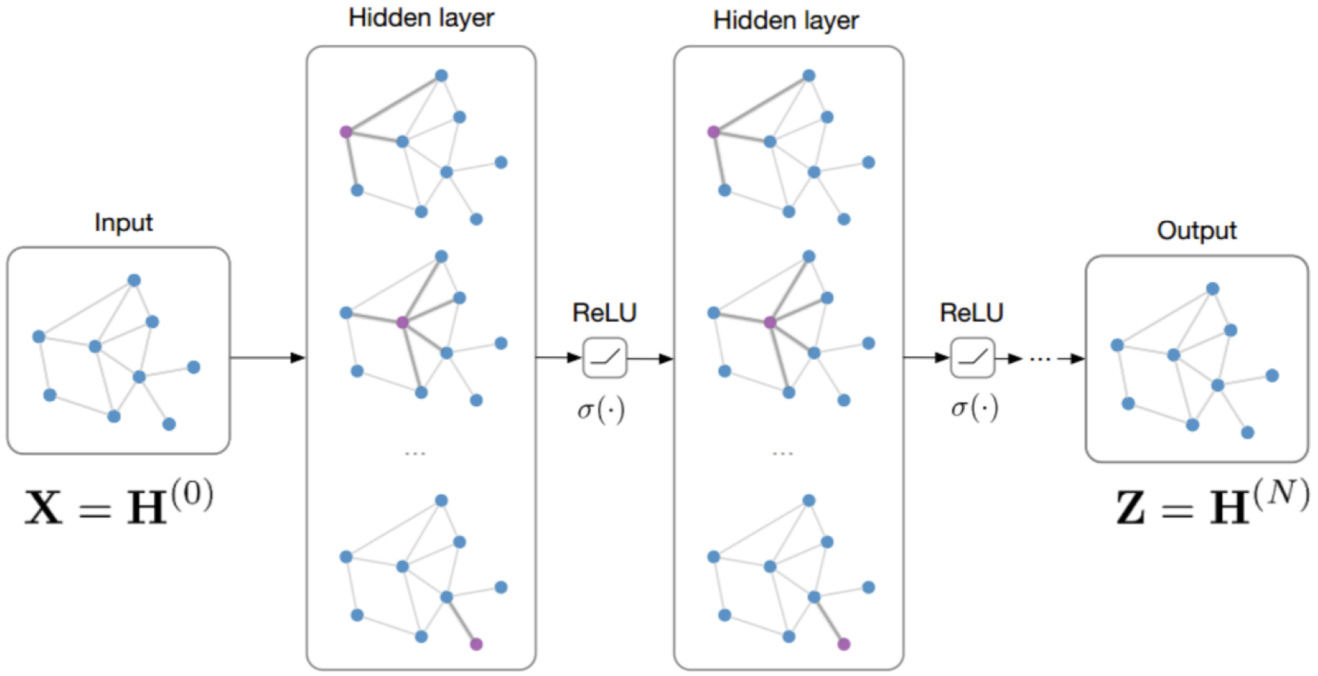
From Shallow to Deep

- So far we have focused on shallow encoders, i.e. embedding lookups:



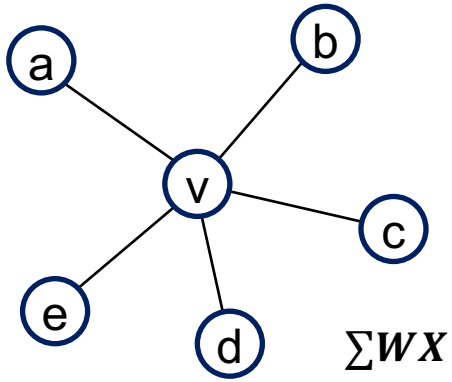
GNN/GCN Model Architecture

- **Input**: preprocess adjacency matrix $\hat{\mathbf{A}}$ and feature matrix $\mathbf{X} \in R^{N \times E}$



- where $\hat{\mathbf{A}} = \tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}$, $\tilde{A} = A + I_N$ is the adjacency matrix of graph G with added self-connections and $\tilde{D}_{ii} = \sum_j \tilde{A}_{ij}$

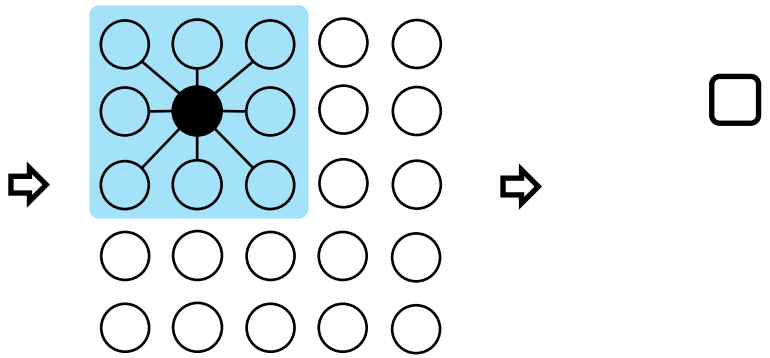
The Core of Graph Neural Networks



$$\boldsymbol{h}_v = f(\boldsymbol{h}_a, \boldsymbol{h}_b, \boldsymbol{h}_c, \boldsymbol{h}_d, \boldsymbol{h}_e)$$

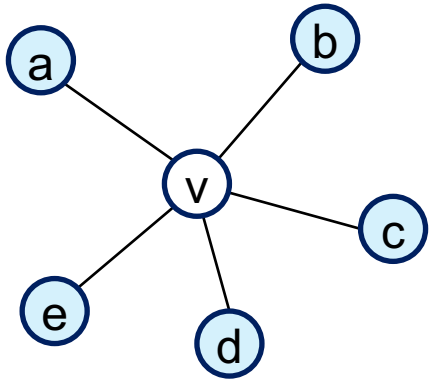
- **Neighborhood Aggregation:**
  - Aggregate neighbor information and pass into a neural network
  - It can be viewed as a center-surround filter in CNN---graph convolutions!

Convolutional neural network



$\sum WX$

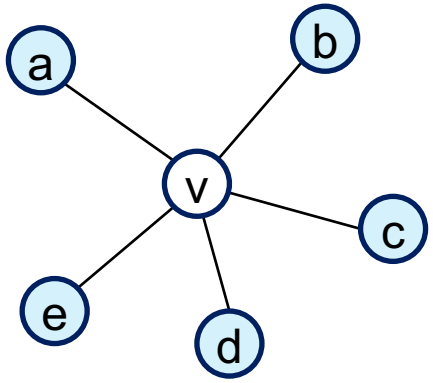
GNN: Graph Convolutional Networks



$$\boldsymbol{h}_v^k = \sigma(\boldsymbol{W}_k \sum_{u \in \mathrm{N}(v) \cup v} \frac{h_u^{k-1}}{\sqrt{|N(u)||N(v)|}})$$

1. Kipf et al. Semi-supervised Classification with Graph Convolutional Networks. ICLR 2017

GNN: Graph Convolutional Networks



parameters in layer k

Non-linear activation function (e.g., ReLU)

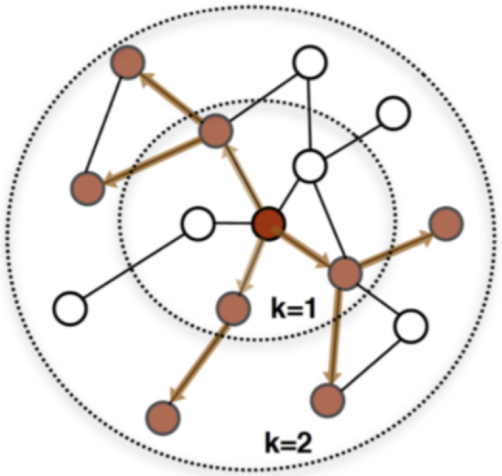
$$\boldsymbol{h}_v^k = \sigma\left(\boldsymbol{W}_k \sum_{u \in \mathrm{N}(v) \cup v} \frac{h_u^{k-1}}{\sqrt{|N(u)||N(v)|}}\right)$$

node v's embedding at layer k

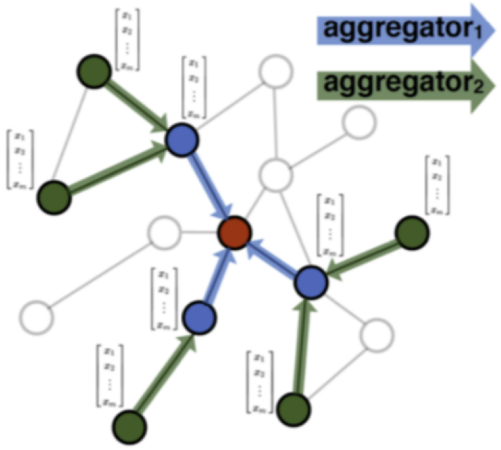
the neighbors of node v

GraphSAGE Model Arthitecture

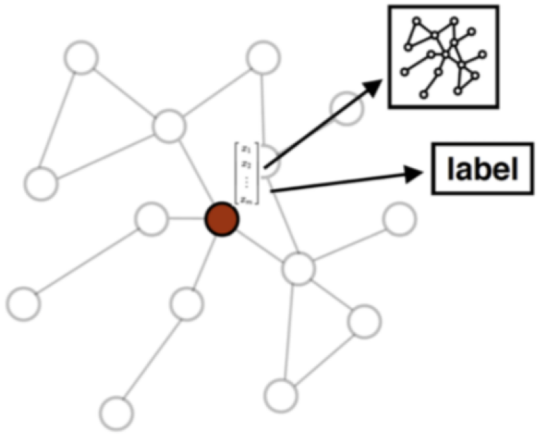
- Idea: Node's neighborhood defines a computation graph.
- Learn how to propagate information across the graph to compute node features



1. Sample neighborhood



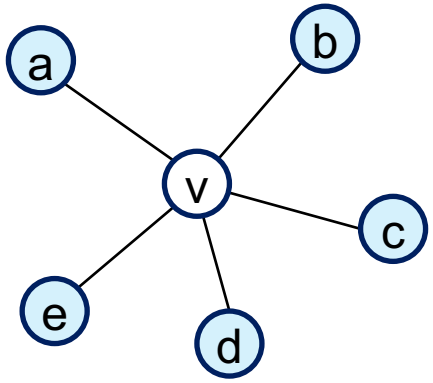
2. Aggregate feature information from neighbors



3. Predict graph context and label using aggregated information

1. Hamilton et al. Inductive Representation Learning on Large Graphs. NIPS 2017

GraphSage



GCN

$$\boldsymbol{h}_v^k = \sigma(\boldsymbol{W}_k \sum_{u \in \mathrm{N}(v) \cup v} \frac{h_u^{k-1}}{\sqrt{|N(u)||N(v)|}})$$

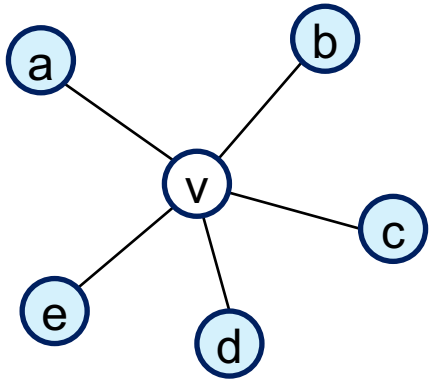
GraphSage

$$\boldsymbol{h}_v^k = \sigma([\boldsymbol{A}_k \cdot \mathrm{AGG}(\{h_u^{k-1}, \forall u \in N(v)\}), \boldsymbol{B}_k h_v^{k-1}])$$

Generalized aggregation: any differentiable function that maps set of vectors to a single vector

1. Hamilton et al. Inductive Representation Learning on Large Graphs. NIPS 2017
2. Slide snipping from "Hamiltion & Tang, AAAI 2019 Tutorial on Graph Representation Learning"

GraphSage



GCN

$$\boldsymbol{h}_v^k = \sigma(\boldsymbol{W}_k \sum_{u \in \mathrm{N}(v) \cup v} \frac{h_u^{k-1}}{\sqrt{|N(u)||N(v)|}})$$

GraphSage

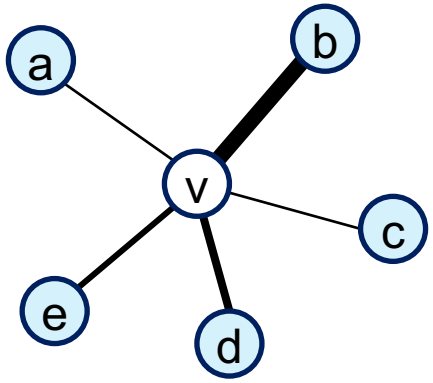
Instead of summation, it concatenate neighbor & self embeddings

$$\boldsymbol{h}_v^k = \sigma([\boldsymbol{A}_k \cdot \mathrm{AGG}(\{h_u^{k-1}, \forall u \in N(v)\}), \boldsymbol{B}_k h_v^{k-1}])$$

Generalized aggregation: any differentiable function that maps set of vectors to a single vector

1. Hamilton et al. Inductive Representation Learning on Large Graphs. NIPS 2017
2. Slide snipping from "Hamiltion & Tang, AAAI 2019 Tutorial on Graph Representation Learning"

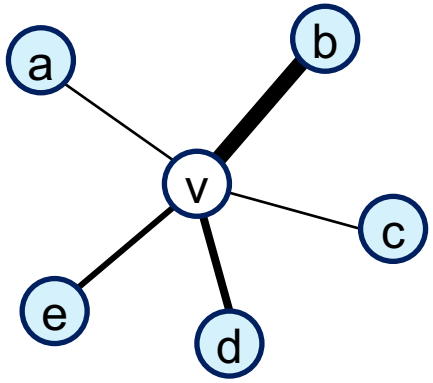
Graph Attention Networks



Realistically, neighbors play different influences

1. Velickovic et al. Graph Attention Networks. ICLR 2018

Graph Attention Networks



GCN

$$\boldsymbol{h}_v^k = \sigma(\boldsymbol{W}_k \sum_{u \in \mathrm{N}(v) \cup v} \frac{h_u^{k-1}}{\sqrt{|N(u)||N(v)|}})$$

Graph Attention

$$\boldsymbol{h}_v^k = \sigma(\sum_{u \in \mathrm{N}(v) \cup v} \alpha_{v,u} \boldsymbol{W}^k h_u^{k-1})$$

Learned attention weights

1. Velickovic et al. Graph Attention Networks. ICLR 2018

GAT Results

Transductive

Method	Cora	Citeseer	Pubmed
MLP	55.1%	46.5%	71.4%
ManiReg (Belkin et al., 2006)	59.5%	60.1%	70.7%
SemiEmb (Weston et al., 2012)	59.0%	59.6%	71.7%
LP (Zhu et al., 2003)	68.0%	45.3%	63.0%
DeepWalk (Perozzi et al., 2014)	67.2%	43.2%	65.3%
ICA (Lu & Getoor, 2003)	75.1%	69.1%	73.9%
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%**
MoNet (Monti et al., 2016)	$81.7 \pm 0.5\%$	—	$78.8 \pm 0.3\%$
GCN-64*	$81.4 \pm 0.5\%$	$70.9 \pm 0.5\%$	**79.0** $\pm 0.3\%$
GAT (ours)	**83.0** $\pm 0.7\%$	**72.5** $\pm 0.7\%$	**79.0** $\pm 0.3\%$

Inductive

Method	PPI
Random	0.396
MLP	0.422
GraphSAGE-GCN (Hamilton et al., 2017)	0.500
GraphSAGE-mean (Hamilton et al., 2017)	0.598
GraphSAGE-LSTM (Hamilton et al., 2017)	0.612
GraphSAGE-pool (Hamilton et al., 2017)	0.600
GraphSAGE*	0.768
Const-GAT (ours)	0.934 ± 0.006
GAT (ours)	**0.973** ± 0.002

- Again, what are the fundamentals underlying the different models?

- GNN: Over-smoothing, Overfitting, Non-robust

GCN can be viewed as multi-layer graph convolution network

- with the following propagation rule

$$H^{(l+1)} = \sigma(\hat{A}H^{(l)}W^{(l)})$$

where $\hat{A} = \widetilde{D}^{-\frac{1}{2}}\widetilde{A}\,\widetilde{D}^{-\frac{1}{2}}$ is the normalized adjacency matrix, $H^{(l)}$ is the $D^{(l)}$-dimensional hidden representation in the l layer.

Graph Convolutional Networks as Signal Rescaling

- Neighborhood aggregation in GCN:

$$H^{(l+1)} = \sigma(\hat{A}H^{(l)}W^{(l)})$$

Node status

influence

- Neighborhood aggregation in NRGCN (for node *i*):

$$H_i^{(l+1)} = \sigma_i^{(l)}[(P^{(l)}\hat{A}Q^{(l)}H^{(l)}W^{(l)})_i]$$

  - *P* and *Q*: diagonal matrix, node ranking-aware rescaling
  - σ_i : node ranking-aware encoder
  - P_{ii}, Q_{ii}, and σ_i are adaptively adjusted according to the network ranking of node i

Network dynamics are driven by nodes' status and influence

Graph Convolutional Networks as Signal Rescaling

- NRGCN layer:

$$H_i^{'} = \sigma_i[(P\hat{A}QHW)_i]$$

- Multi-head Propagation mechanism:

$$H_i^{'} = \Big\|_{k=1}^{K} \sigma_i^{(k)}[(P^{(k)}\hat{A}Q^{(k)}HW^{(k)})_i]$$

- Multi-hop variants:

$$H_i^{'} = \sigma_i[(P\hat{A}^k QHW)_i]$$

Generalization to Graph Attention

- When *P* normalizes signals in different range, the model can function as node, edge, and path attention mechanisms

(Node attention)

$$\begin{cases} S = \hat{A}Q \\ \vec{p}_i = P_{ii} = \dfrac{1}{\vec{q}^T\vec{1}} \end{cases}$$

(Edge attention)

$$\begin{cases} S = \hat{A}Q \\ \vec{p} = \dfrac{1}{S\vec{1}} \end{cases}$$

(K-hop edge attention)

$$\begin{cases} S = \hat{A}^k Q \\ \vec{p} = \dfrac{1}{S\vec{1}} \end{cases}$$

(Path attention)

$$\begin{cases} S = \hat{A}Q_k\hat{A}Q_{k-1}\ldots\hat{A}Q_1 \\ \vec{p} = \dfrac{1}{S\vec{1}} \end{cases}$$

GAT can be considered as a special case of NRGCN

GCN, GAT

- GCN

$$\mathbf{H}' = \sigma(\mathcal{L}\mathbf{H}\mathbf{W})$$

Rescale
Re-normalize
Propagate

- GAT

$$\begin{cases} \mathbf{H}' = \sigma\left(\mathcal{N}\left(\mathbf{P}\mathcal{L} + \mathcal{L}\mathbf{Q}\right)\mathbf{H}\mathbf{W}\right) \\ \mathcal{L} = A + I_N \\ \mathcal{N}(\cdot) = \text{SparseRowSoftmax}(\text{LeakyReLU}(\cdot)) \\ \mathbf{P}_{ii} = \left(\mathbf{H}\mathbf{W}\vec{p}\right)_i,\ \mathbf{Q}_{ii} = \left(\mathbf{H}\mathbf{W}\vec{q}\right)_i \end{cases}$$

- ASGCN

$$\begin{cases} \mathbf{H}' = \sigma\left(\mathcal{N}\left(\mathcal{L}\mathbf{Q}\right)\mathbf{H}\mathbf{W}\right) \\ \mathcal{N}(\mathbf{M}) = \frac{1}{n}\mathbf{M} \\ \mathbf{Q}_{ii} = \frac{q_i}{q^*(u_i)},\ q_i \sim \text{Ber}(n, q^*(u_i)) \end{cases}$$

GraphSAGE, FastGCN

- GraphSAGE

$$\begin{cases} \mathbf{H}' = \sigma\left(\mathcal{N}\left(\mathcal{L} \odot \mathbf{Q}\right)\mathbf{H}\mathbf{W}\right) \\ \mathcal{L} = A + I_N \\ \mathcal{N}(\mathbf{M}) = D^{-1}\mathbf{M},\ D_{ii} = \sum_j \mathbf{M}_{ij} \\ \left\{\mathbf{Q}_{ij} | \hat{A}_{ij} \neq 0\right\} \sim \text{Sample}\left(\deg(i), S_l\right) \end{cases}$$

- FastGCN

$$\begin{cases} \mathbf{H}' = \sigma\left(\mathcal{N}\left(\mathcal{L}\mathbf{Q}\right)\mathbf{H}\mathbf{W}\right) \\ \mathcal{N}(\mathbf{M}) = \dfrac{1}{t_l}\mathbf{M} \\ \{q(u_1)\mathbf{Q}_{11}, q(u_2)\mathbf{Q}_{22}, \cdots, q(u_n)\mathbf{Q}_{nn}\} \sim \text{Sample}(N, t_l) \end{cases}$$

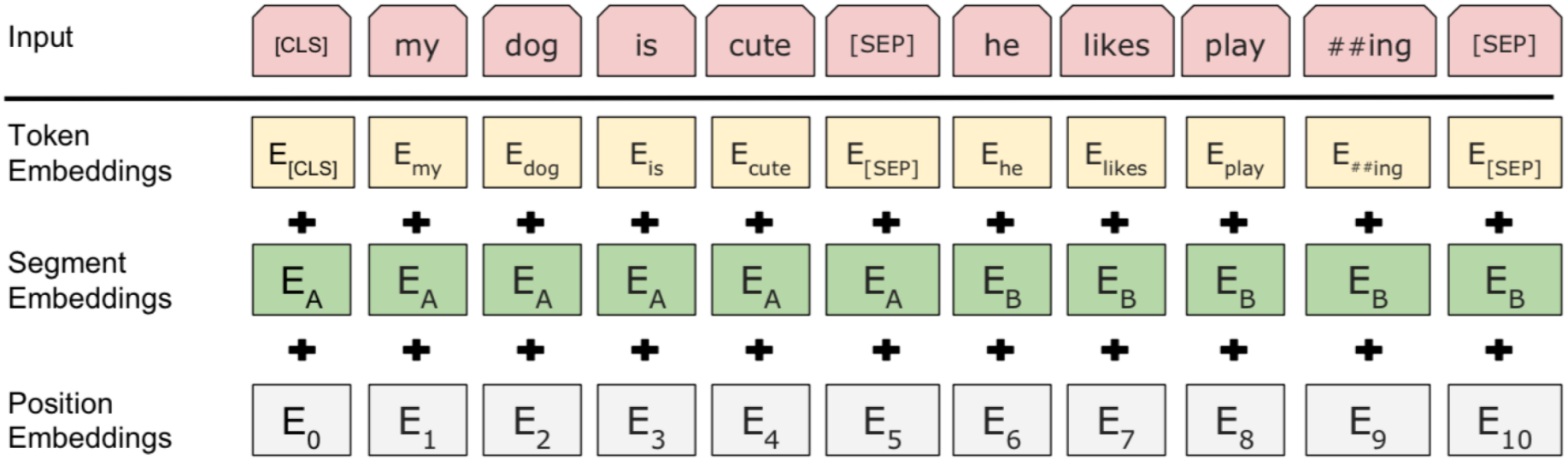
Graph Convolutional Networks as Signal Rescaling

Table 1. GCNs as Signal Rescaling (Note that $\mathbf{P}, \mathbf{Q}, \mathcal{N}(\cdot)$ are model specified).

Methods	Rescaling and Propagation Rules
vanilla GCN	$\mathbf{H}' = \sigma\left(\mathcal{L}\mathbf{H}\mathbf{W}\right)$
GAT	$\mathbf{H}' = \sigma\left(\mathcal{N}\left(\mathbf{P}\mathcal{L} + \mathcal{L}\mathbf{Q}\right)\mathbf{H}\mathbf{W}\right)$
$\text{GraphSAGE}_{\text{mean}}$	$\mathbf{H}' = \sigma\left(\mathcal{N}\left(\mathcal{L} \odot \mathbf{Q}\right)\mathbf{H}\mathbf{W}\right)$
FastGCN	$\mathbf{H}' = \sigma\left(\mathcal{N}\left(\mathcal{L}\mathbf{Q}\right)\mathbf{H}\mathbf{W}\right)$
ASGCN	$\mathbf{H}' = \sigma\left(\mathcal{N}\left(\mathcal{L}\mathbf{Q}\right)\mathbf{H}\mathbf{W}\right)$

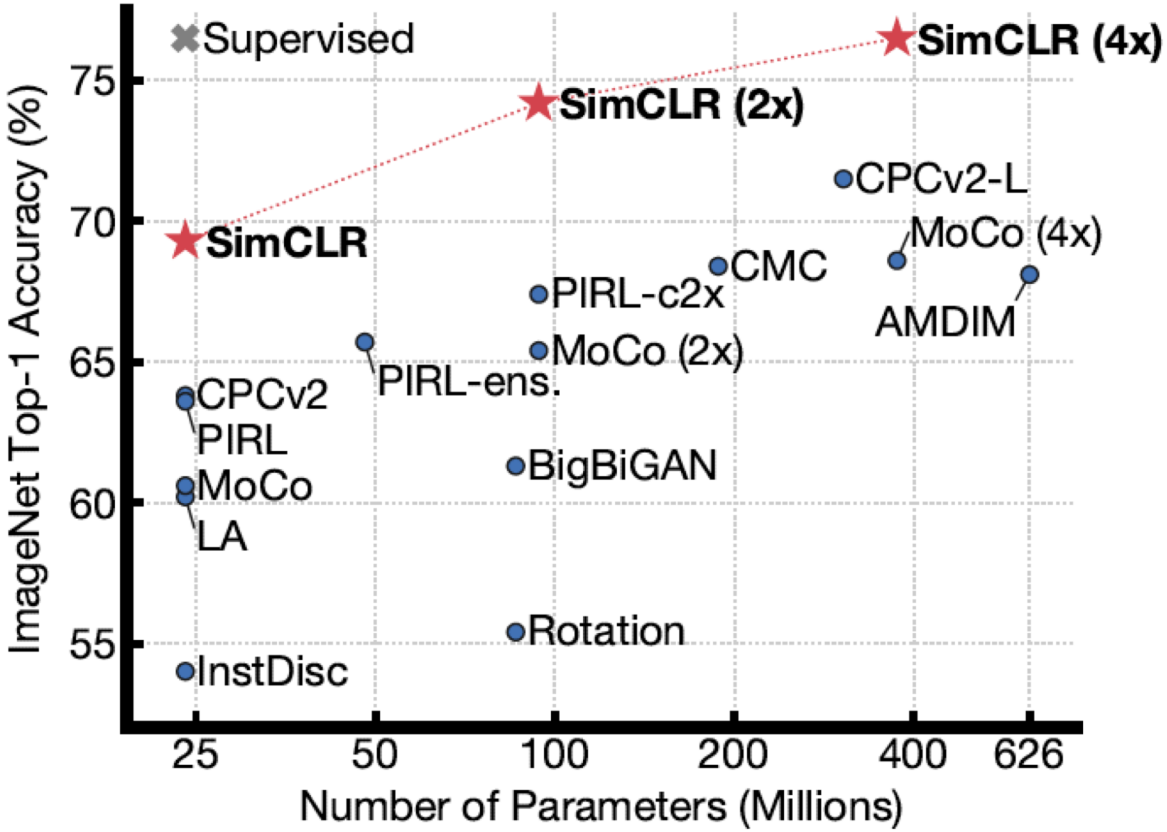
Category	Method	Cora	Citeseer	Pubmed
Non-GCN Methods	MLP	55.1	46.5	71.4
	ManiReg	59.5	60.1	70.7
	SemiEmb	59.0	59.6	71.1
	LP	68.0	45.3	63.0
	DeepWalk	67.2	43.2	65.3
	ICA	75.1	69.1	73.9
	Planetoid	75.7	64.7	77.2
Graph Convolution	Chebyshev	81.2	69.8	74.4
	GCN	81.5	70.3	79.0
	MixHop	81.9±0.4	71.4±0.8	**80.8±0.6**
	FastGCN*	80.0±0.6	69.5±0.6	77.8±0.4
	ASGCN*	78.5±0.5	68.9±0.5	75.5±0.4
	GAT	83.0±0.7	72.5±0.7	79.0±0.3
	GAT-SR**	83.4±0.4	72.4±0.6	78.7±0.4
	GAT-16**	83.4±0.4	72.3±0.6	78.8±0.3
	SRGCN	**84.1±0.5**	**73.4±0.7**	79.5±0.4
	SRGCN (Pre)	83.8±0.6	73.2±0.6	79.3±0.6
	SRGCN (Post)	**84.1±0.5**	73.3±0.7	79.4±0.5
	SRGCN (1/2)	83.9±0.6	73.3±0.9	79.3±0.6
	SRGCN (1/4)	84.0±0.6	73.0±0.9	79.0±0.8
	SRGCN (1/8)	84.0±0.6	72.5±1.4	77.5±1.3
p-value (SRGCN vs. GAT-16)		5.8e-21	1.4e-25	5.1e-29

BERT



- Pre-train
- Fine tune
- Beat all state-of-the-arts on 11 NLP tasks in 2018
- BERTology: XLNet, Roberta, ALBert, TinyBERT, etc.

Contrastive Learning: MoCo, SimCLR, etc.



- Simplified contrastive learning framework
- Outperform previous self-supervised and semi-supervised methods on ImageNet

https://arxiv.org/abs/2002.05709

Challenges

- How to combine Graph with Pre-Training (BERT/CL)?
- GNN: Over-smoothing, Overfitting, Non-robust

GNN+推理...

SEARCH

Let us start with a challenging question

—Multi-hop Question Answering (QA)

认知图谱：算法与认知的结合

Question: Who is the director of the 2003 film which has scenes in it filmed at the Quality Cafe in Los Angeles?

Quality Café

The Quality Cafe is a now-defunct diner in Los Angeles, California. The restaurant has appeared as a location featured in a number of Hollywood films, including Old School, Gone in 60 Seconds, ...

Los Angeles

Los Angeles is the most populous city in California, the second most populous city in the United States, after New York City, and the third most populous city in North America.

Alessandro Moschitti

Alessandro Moschitti is a professor of the CS Department of the University of Trento, Italy. He is currently a Principal Research Scientist of the Qatar Computing Research Institute (QCRI)

WIKIPEDIA
The Free Encyclopedia

Old School

Old School is a 2003 American comedy film released by Dream Works Pictures and The Montecito Picture Company and directed by Todd Phillips.

Todd Phillips

Todd Phillips is an American director, producer, screenwriter, and actor. He is best known for writing and directing films, including Road Trip (2000), Old School (2003), Starsky & Hutch (2004), and The Hangover Trilogy.

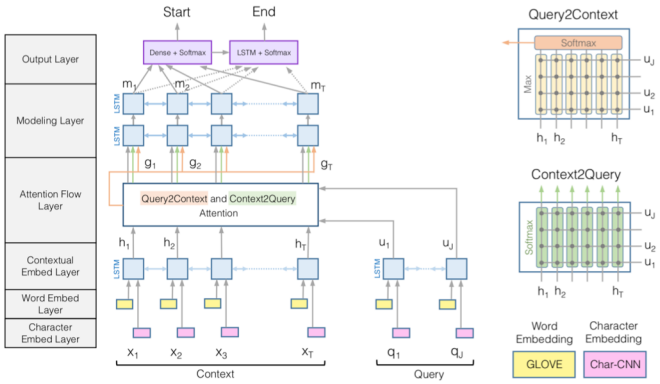
Tsinghua University

Tsinghua University is a major research university in Beijing and dedicated to academic excellence and global development. Tsinghua is perennially ranked as one of the top academic institutions in China, Asia, and worldwide...

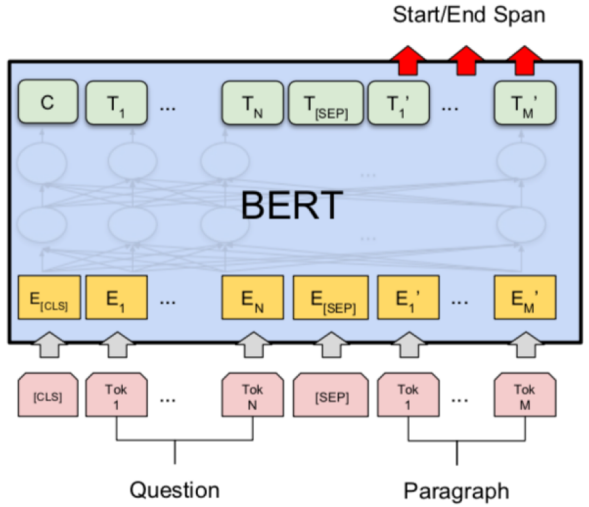
算法：BIDAF, BERT, XLNet

- 目标：理解整个文档，而不仅仅是局部片段
- 但仍然缺乏在知识层面上的推理能力

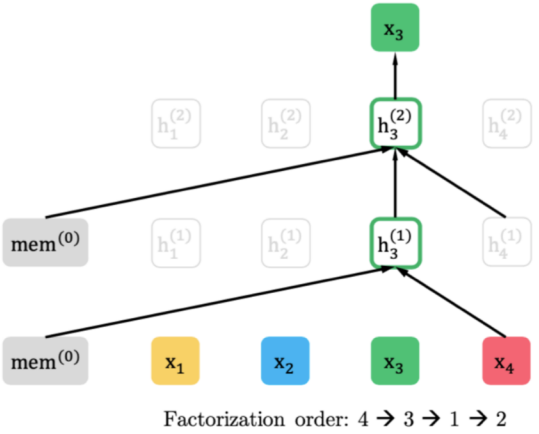
BiDAF



BERT



XLNet

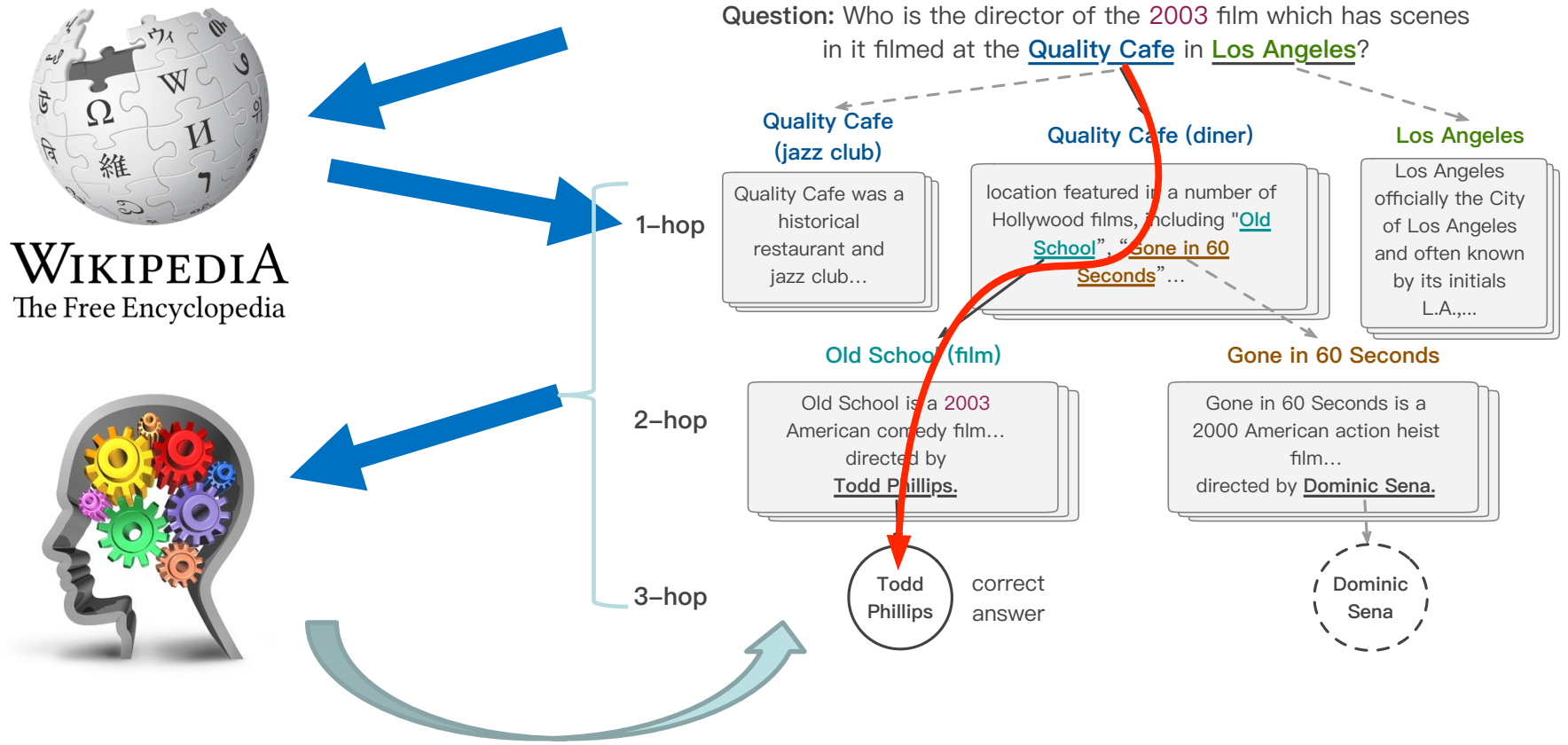


挑战：可解释性

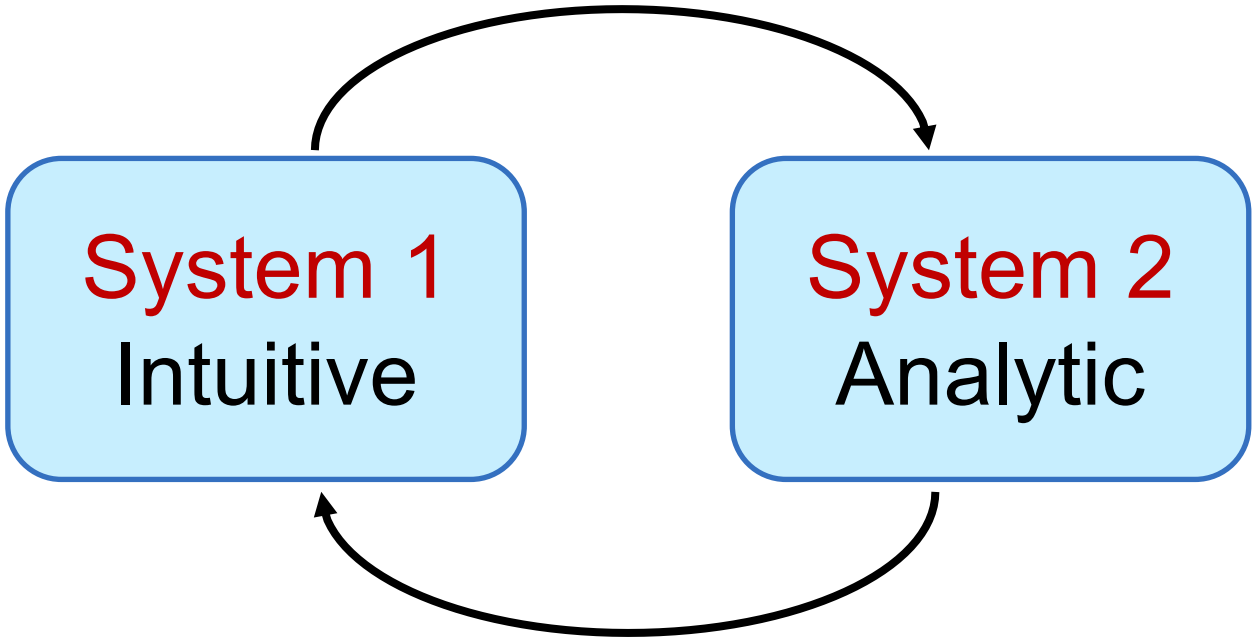
- 大部分阅读理解方法都只能看做**黑盒**：
  - 输入：问题和文档
  - 输出：答案文本块（在文档中的起止位置）

- 如何让用户可以验证答案的对错：
  - 推理路径或者子图
  - 每个推理节点上的支撑事实
  - 用于对比的其他可能答案和推理路径

认知图谱：知识表示，推理和决策



和认知科学的结合



Dual Process Theory (Cognitive Science)

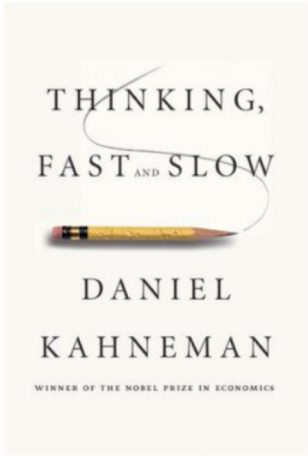
SYSTEM 1 VS. SYSTEM 2 COGNITION

2 systems (and categories of cognitive tasks):

Manipulates high-level / semantic concepts, which can be recombined combinatorially

System 1

- Intuitive, fast, **UNCONSCIOUS**, non-linguistic, habitual
- Current DL



System 2

- Slow, logical, sequential, **CONSCIOUS**, linguistic, algorithmic, planning, reasoning
- Future DL

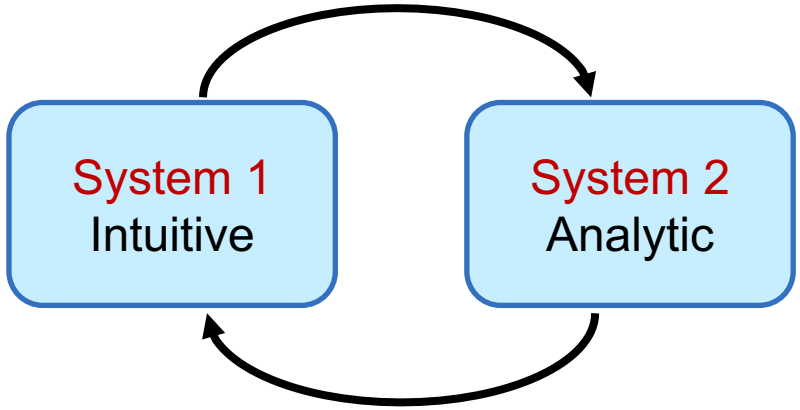
Mila

3

1. From Bengio's NIPS'2019 Keynote

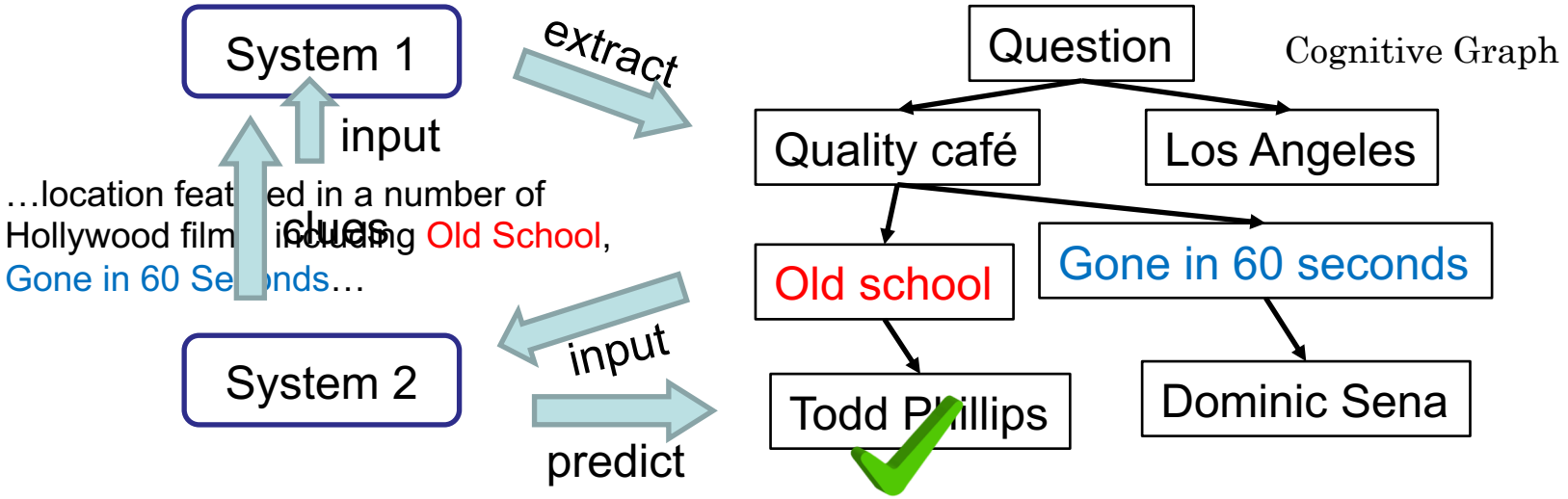
Reasoning w/ Cognitive Graph

- System 1:
  - Knowledge expansion by association in text when reading
- System 2:
  - Decision making w/ all the information



CogQA: Cognitive Graph for QA

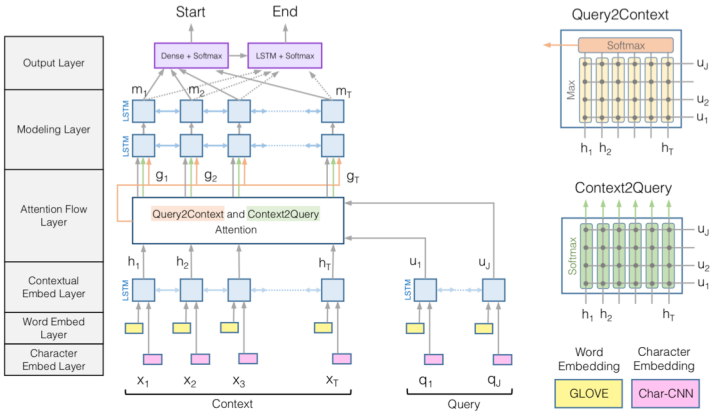
- An iterative framework corresponding to dual process theory
- System 1
  - extract entities to build the cognitive graph
  - generate semantic vectors for each node
- System 2
  - Do reasoning based on semantic vectors and graph
  - Feed clues to System 1 to extract next-hop entities



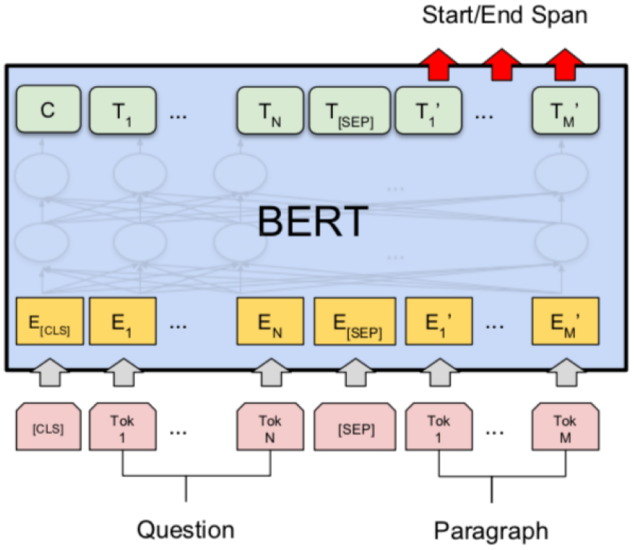
System 1: BIDAF, BERT

- reading comprehension: target at understanding the whole paragraph

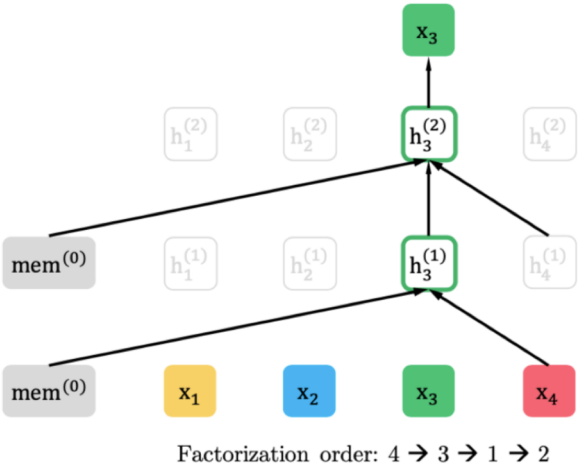
BiDAF



BERT

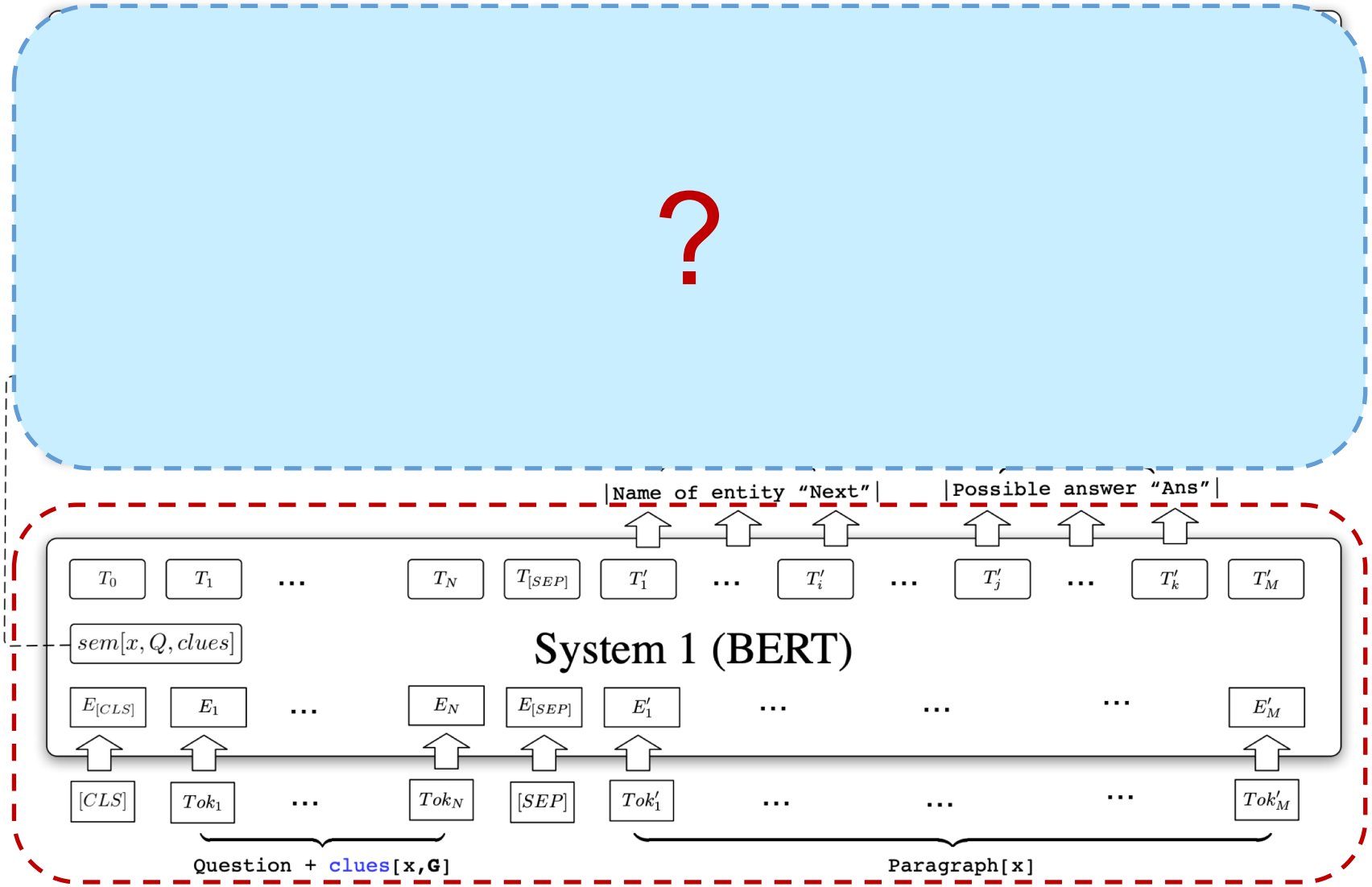


XLNet



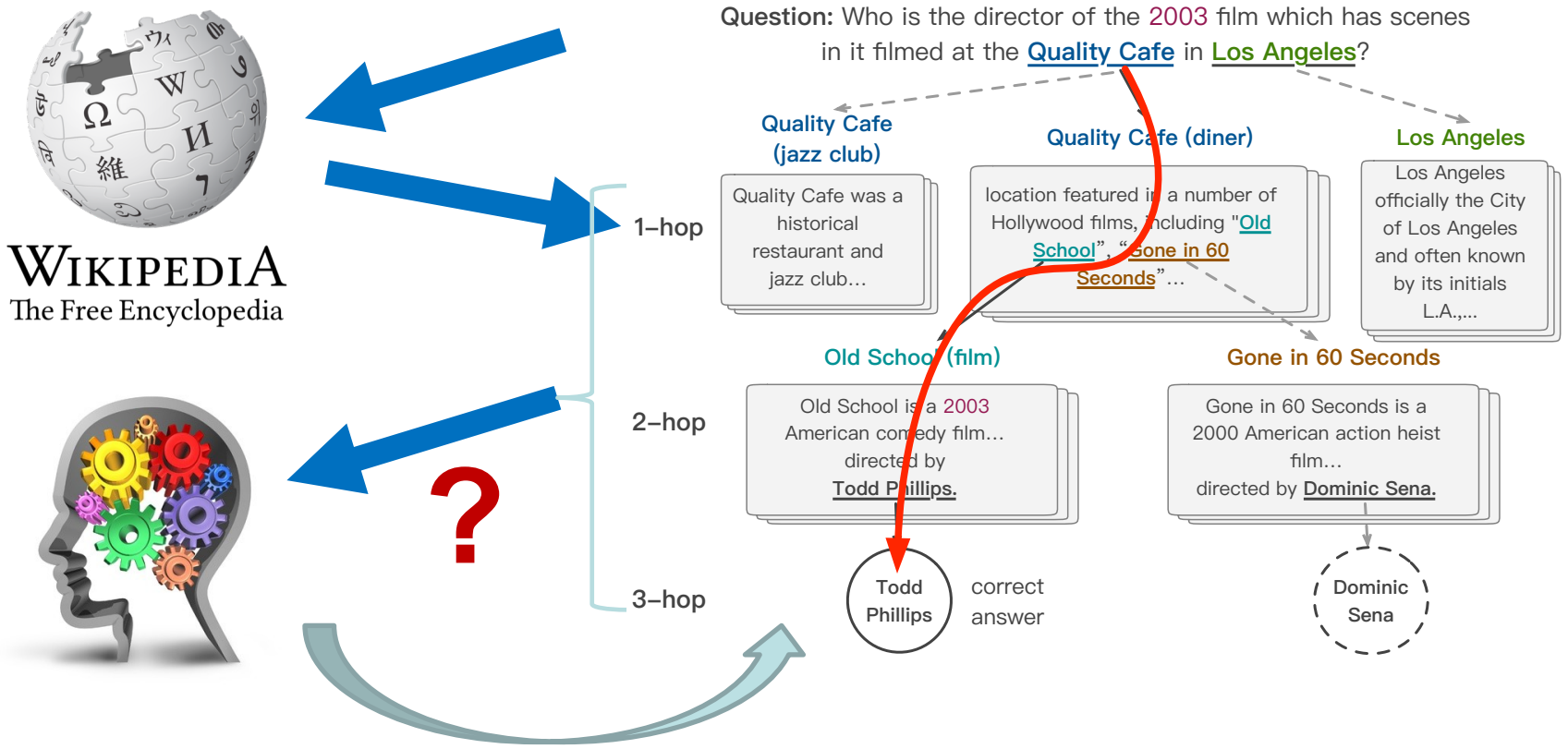
1. Rajpurkar, Pranav, et al. "SQuAD: 100,000+ Questions for Machine Comprehension of Text." EMNLP. 2016.

Cognitive Graph: DL + Dual Process Theory

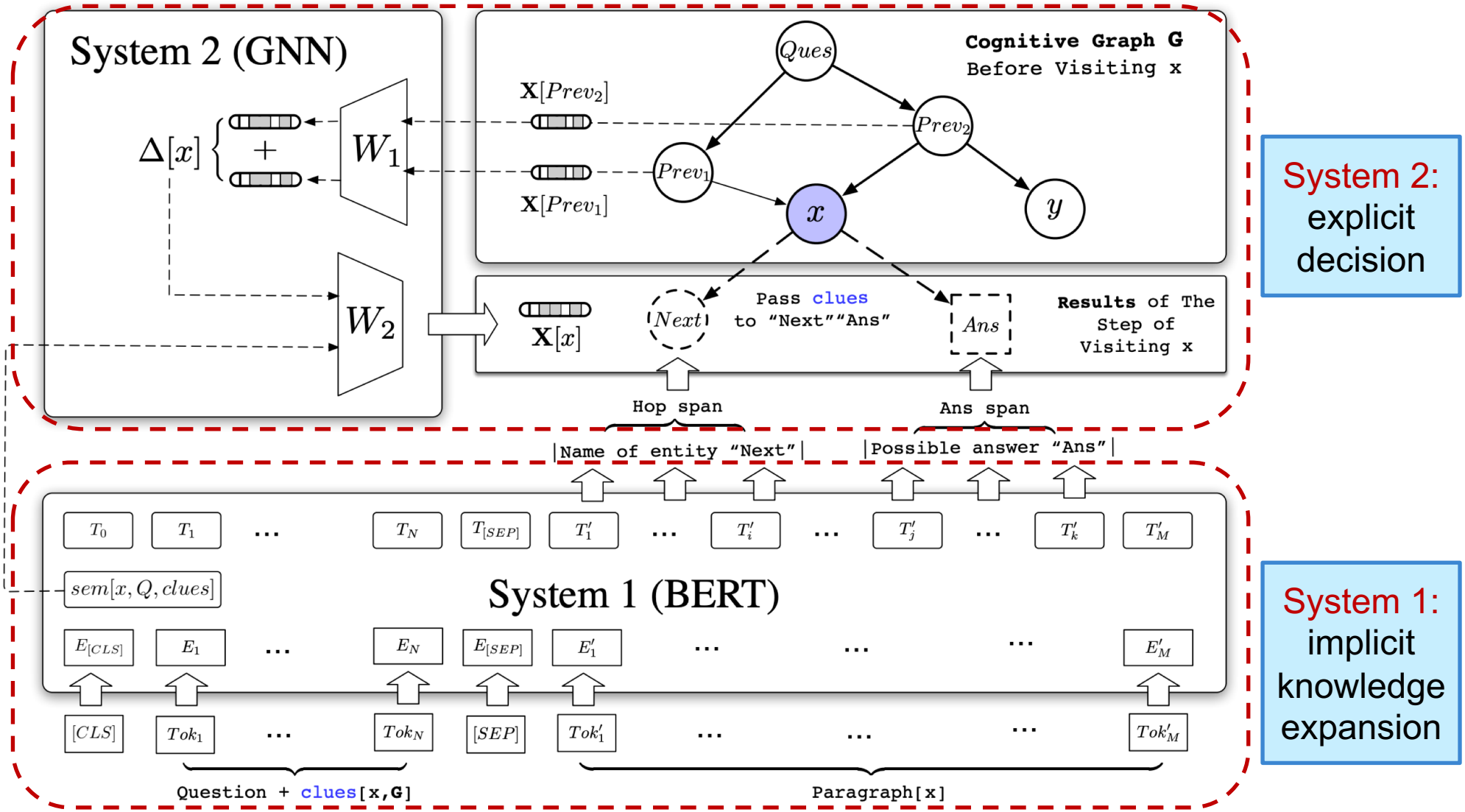


1. M. Ding, C. Zhou, Q. Chen, H. Yang, and J. Tang. Cognitive Graph for Multi-Hop Reading Comprehension at Scale. ACL'19.

System 2: Reasoning, and Decision

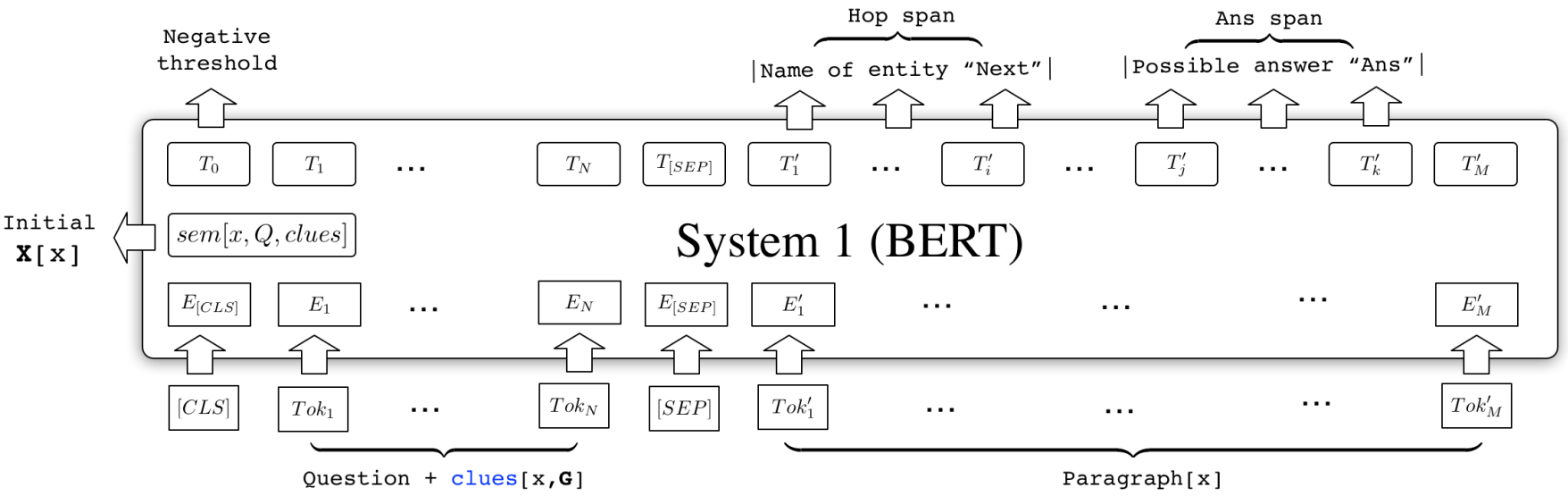


Cognitive Graph: DL + Dual Process Theory



1. M. Ding, C. Zhou, Q. Chen, H. Yang, and J. Tang. Cognitive Graph for Multi-Hop Reading Comprehension at Scale. ACL'19.

System 1: the BERT Implementation



$$[CLS]\ Question\ [SEP]\ clues[x, \mathcal{G}]\ [SEP] \quad Para[x]$$

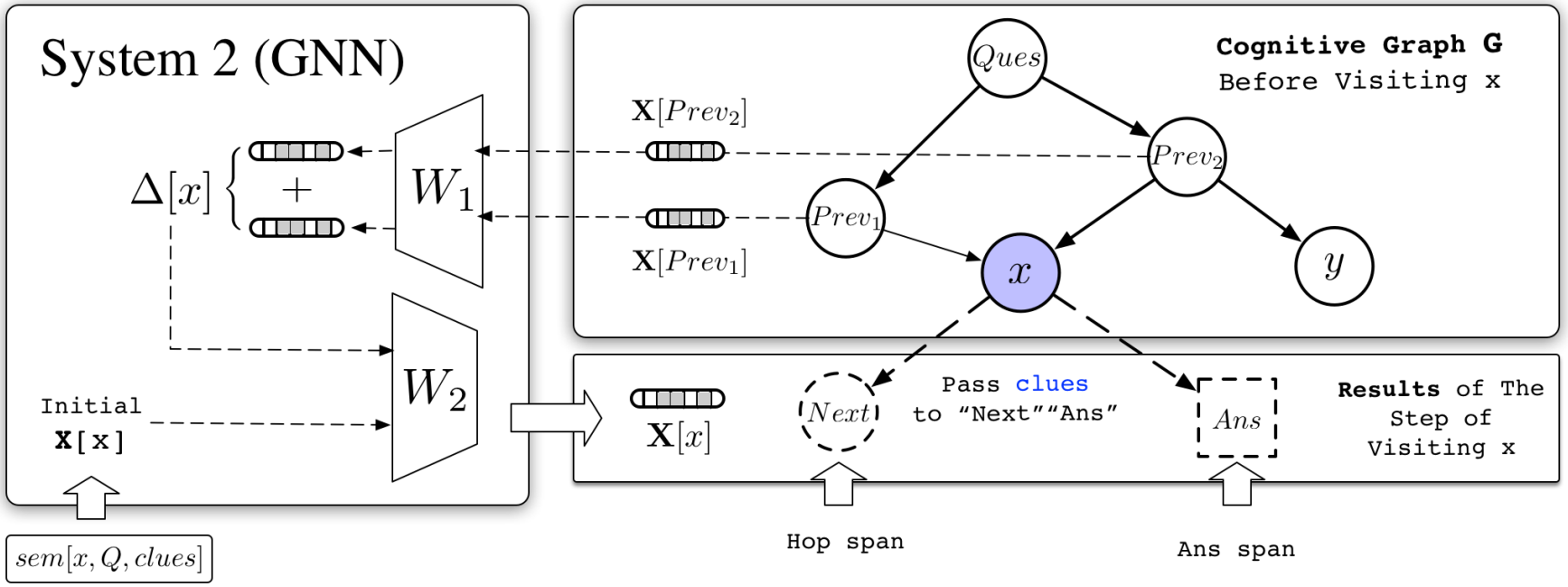
Sentence A Sentence B

$$P_{ans}^{start}[i] = \frac{e^{\mathbf{S}_{ans} \cdot \mathbf{T}_i}}{\sum_j e^{\mathbf{S}_{ans} \cdot \mathbf{T}_j}}$$

$$end_k = \underset{start_k \le j \le start_k + maxL}{\arg\max} P_{ans}^{end}[j]$$

- Extract top-k next-hop entities and answer candidates respectively
  - Predict the start and end probabilities of each position
- Generate semantic vectors for entities based on their documents
- Take the 0-th probability as negative threshold
  - Ignore the spans whose start probabilities are small than the negative threshold

System 2: the GNN implementation



At each step, hidden representations $\mathbf{X}$ for nodes are updated according to the propagation rules:

$$\Delta = \sigma((AD^{-1})^T \sigma(\mathbf{X}W_1))$$
$$\mathbf{X}' = \sigma(\mathbf{X}W_2 + \Delta)$$

Predictor $\mathcal{F}$ is a two-layer MLP, which predicts the final answer based on hidden representations $\mathbf{X}$:

$$answer = \underset{\text{answer node } x}{\arg\max}\ \mathcal{F}(\mathbf{X}[x])$$

Performance

- HotpotQA is a dataset with leaderboard similar to SQuAD
- CogQA ranked 1st from 21, Feb to 15, May (nearly 3 month)

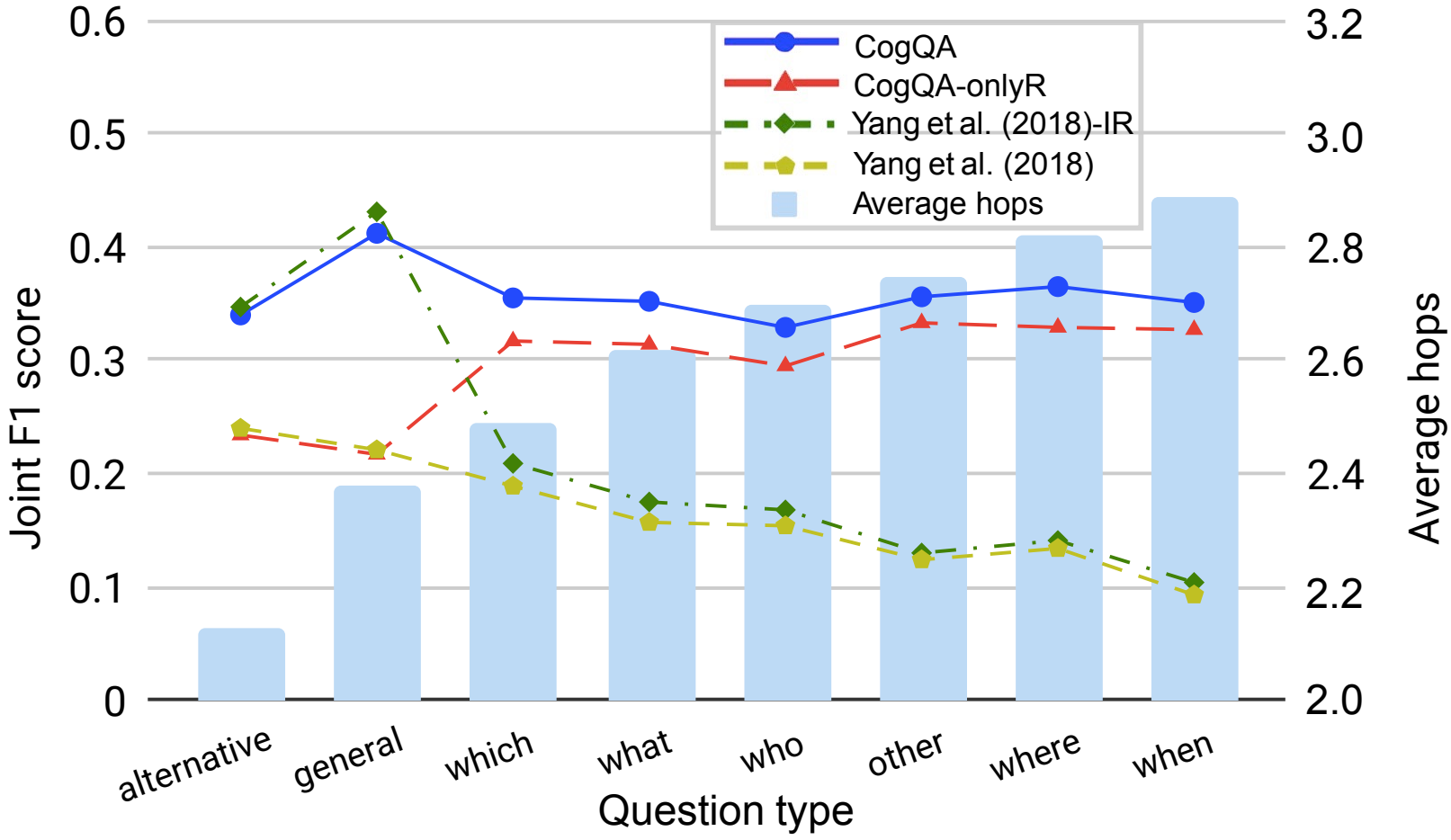
	Model	Ans				Sup				Joint			
		EM	F_1	Prec	Recall	EM	F_1	Prec	Recall	EM	F_1	Prec	Recall
Dev	Yang et al. (2018)	23.9	32.9	34.9	33.9	5.1	40.9	47.2	40.8	2.5	17.2	20.4	17.8
	Yang et al. (2018)-IR	24.6	34.0	35.7	34.8	10.9	49.3	52.5	52.1	5.2	21.1	22.7	23.2
	BERT	22.7	31.6	33.4	31.9	6.5	42.4	54.6	38.7	3.1	17.8	24.3	16.2
	CogQA-sys1	33.6	45.0	47.6	45.4	**23.7**	58.3	**67.3**	56.2	12.3	32.5	39.0	31.8
	CogQA-onlyR	34.6	46.2	48.8	46.7	14.7	48.2	56.4	47.7	8.3	29.9	36.2	30.1
	CogQA-onlyQ	30.7	40.4	42.9	40.7	23.4	49.9	56.5	48.5	**12.4**	30.1	35.2	29.9
	CogQA	**37.6**	**49.4**	**52.2**	**49.9**	23.1	**58.5**	64.3	**59.7**	12.2	**35.3**	**40.3**	**36.5**
Test	Yang et al. (2018)	24.0	32.9	-	-	3.86	37.7	-	-	1.9	16.2	-	-
	QFE	28.7	38.1	-	-	14.2	44.4	-	-	8.7	23.1	-	-
	DecompRC	30.0	40.7	-	-	N/A	N/A	-	-	N/A	N/A	-	-
	MultiQA	30.7	40.2	-	-	N/A	N/A	-	-	N/A	N/A	-	-
	GRN	27.3	36.5	-	-	12.2	48.8	-	-	7.4	23.6	-	-
	CogQA	**37.1**	**48.9**	-	-	**22.8**	**57.7**	-	-	**12.4**	**34.9**	-	-

Table 1: Results on HotpotQA (fullwiki setting). The test set is not public. The maintainer of HotpotQA only offers EM and F_1 for every submission. N/A means the model cannot find supporting facts.

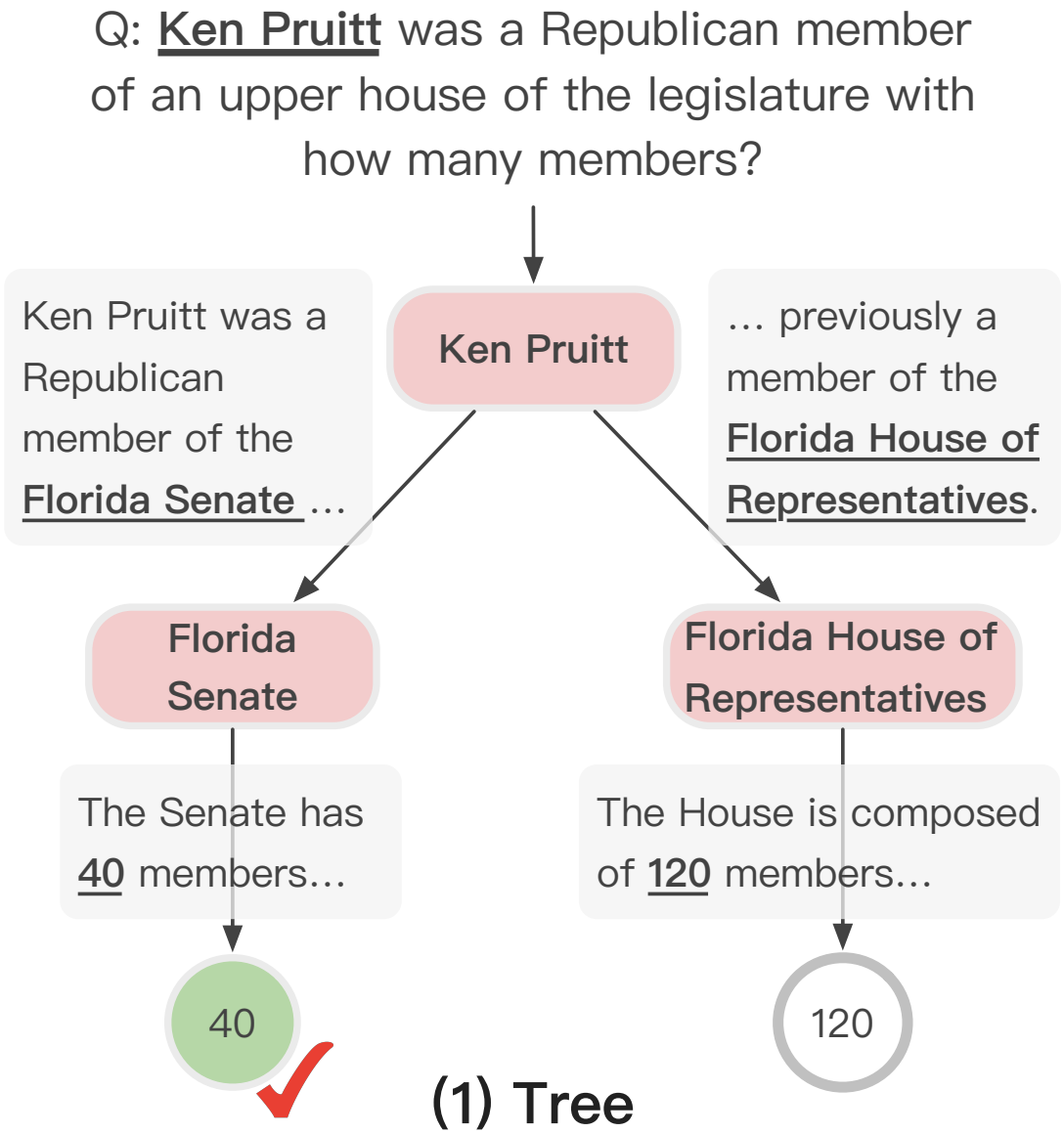
** Code available at https://github.com/THUDM/CogQA

Reasoning Power

CogQA Performs much better on question with more hops !



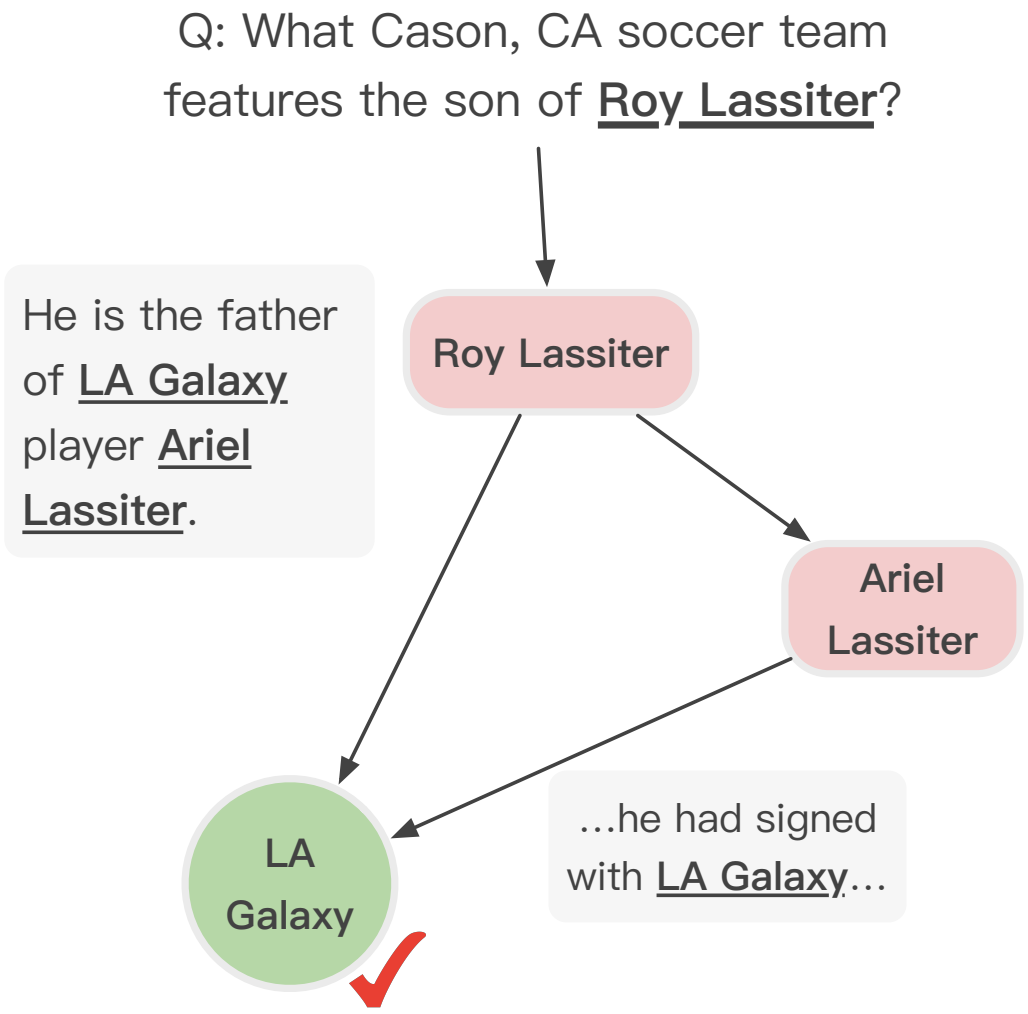
Case Study



(1) Tree

- Tree-shape Cognitive Graph
- Users can verify the answer by comparing it with another possible reasoning chain.
- "*Upper House*" in the question is similar to "*Senate*" not "*House of Representative*"

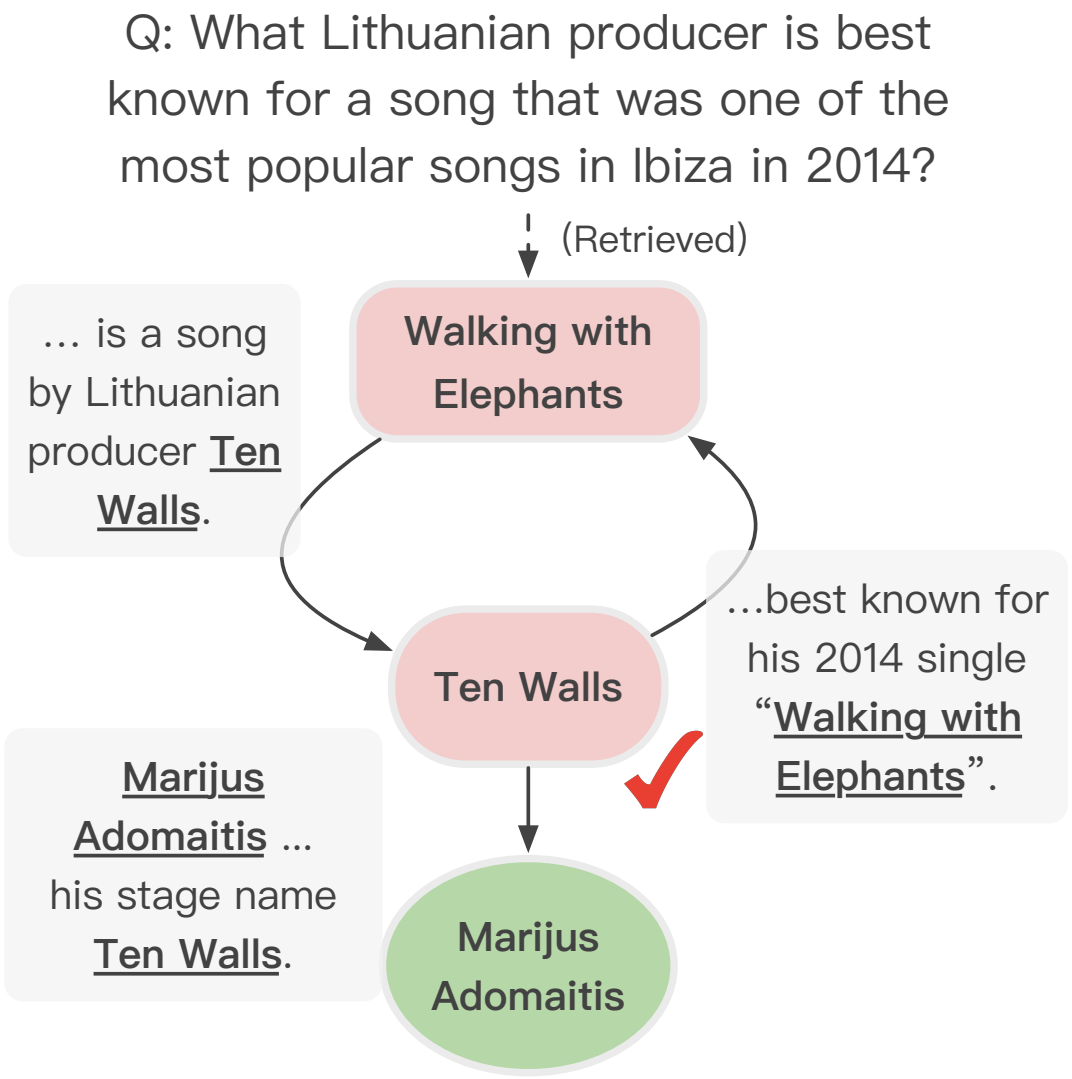
Case Study



(2) DAG

- DAG-shape Cognitive Graph
- Multiple supporting facts provides richer information, increasing the credibility of the answer.

Case Study



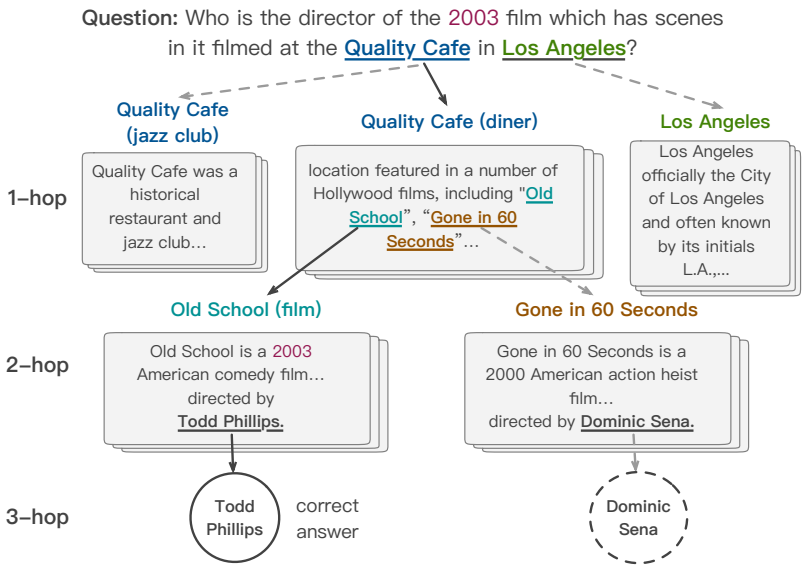
(3) Cyclic Graph

- CogQA gives the answer "Marijus Adomaitis" while the ground truth is "Ten Walls".
- By examining, Ten Walls is just the stage name of Marijus Adomaitis!
- Without cognitive graphs, black-box models cannot achieve it.

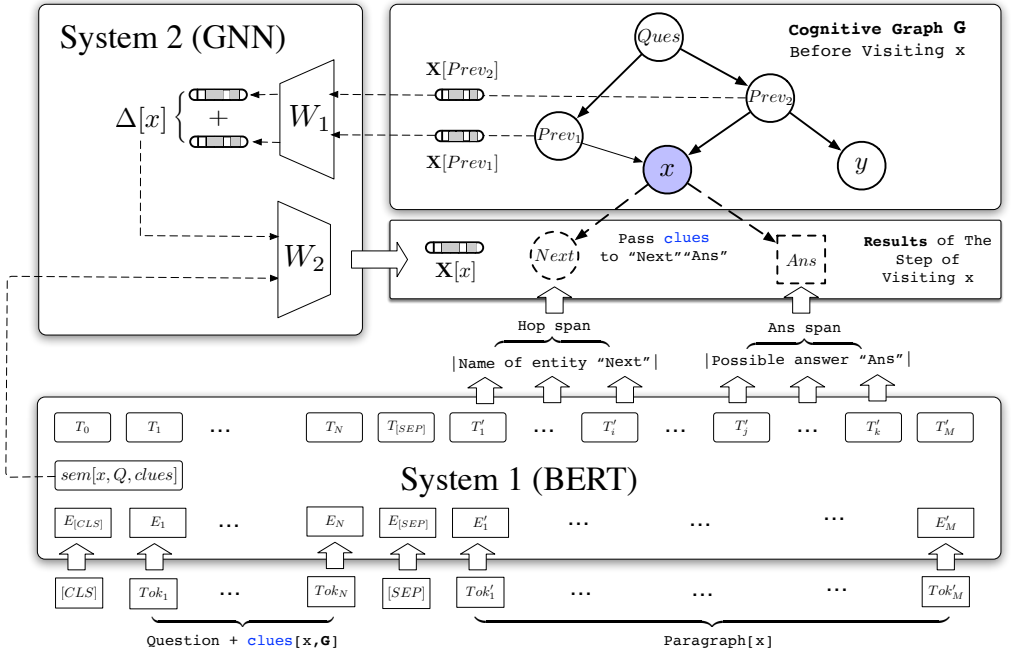
Summary

- Iterative Framework --> Myopic Retrieval
- Cognitive Graph --> Explainability
- Dual process theory --> System 2 Reasoning

Cognitive graph

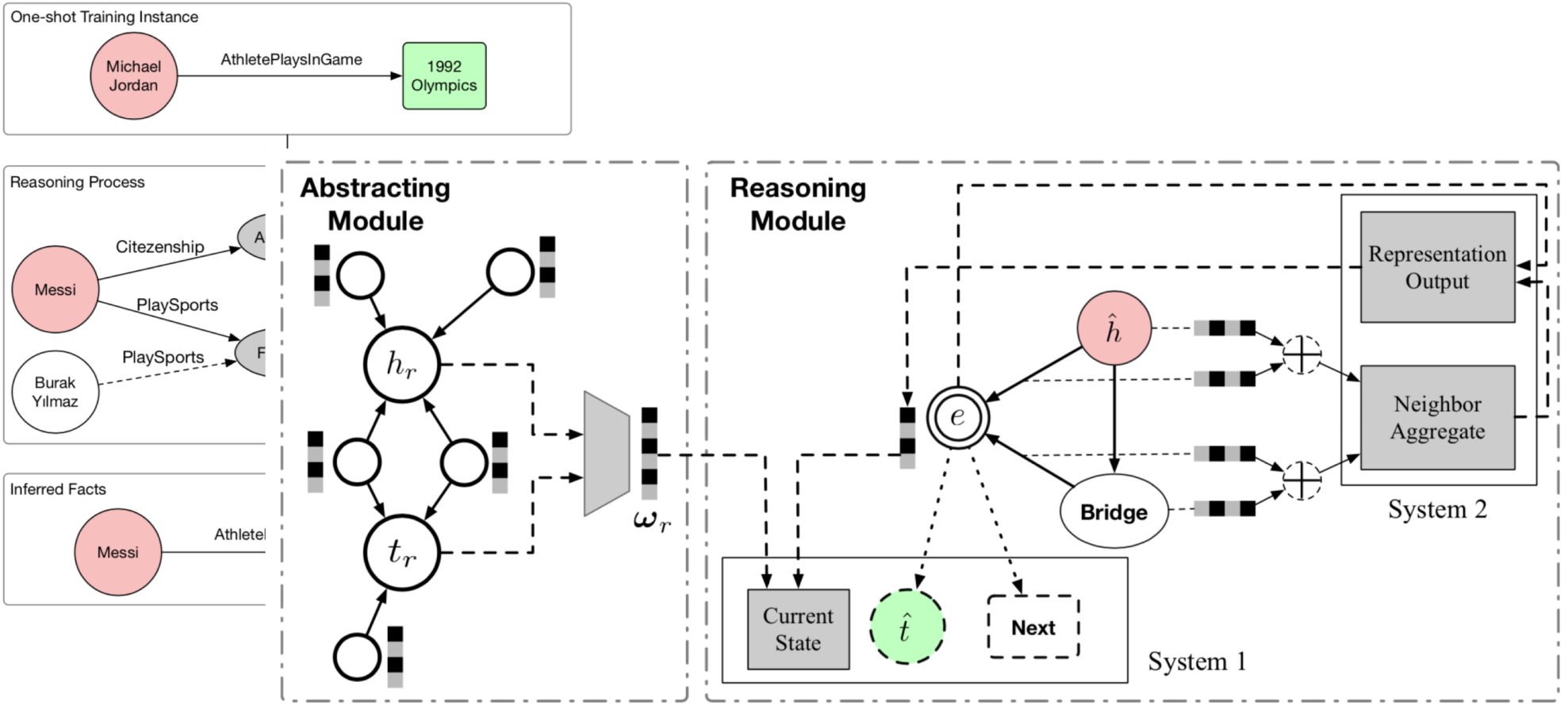


CogQA framework



More Applications: KG completion

- Completing knowledge graph with cognitive graph



挑战与未来…

第三代人工智能的理论体系

- 早在2015年，张钹老师就提出第三代人工智能体系的雏形；2017年DARPA发起XAI项目，从可解释的机器学习系统、人机交互技术以及可解释的心理学理论三个方面，全面开展可解释性AI系统的研究
- 2018年底，正式公开提出**第三代人工智能的理论框架体系**
  - 建立**可解释、鲁棒性**的人工智能理论和方法
  - 发展**安全、可靠、可信及可扩展**的人工智能技术
  - 推动人工智能**创新**应用
- 具体实施路线图
  - 与**脑科学**融合，发展脑启发的人工智能理论
  - **数据与知识融合**的人工智能理论与方法
- 第三代人工智能的理念在国内外获得广泛影响力

挑战与未来

Edward Feigenbaum
Turing Award Winner

认知与推理

—Trillion-scale common-sense knowledge graph

Tim Berners Lee
Turing Award Winner

Big Data ⇨ Knowledge ⇨ Intelligence

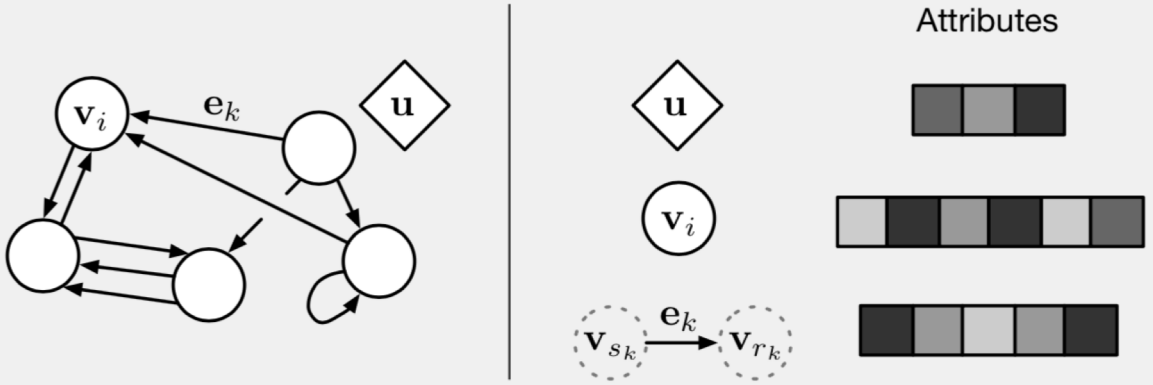
* AI = Knowledge + Intelligence

1. J. Tang, J. Zhang, L. Yao, J. Li, L. Zhang, and Z. Su. ArnetMiner: Extraction and Mining of Academic Social Networks. KDD'08. pp.990-998.

graph_net

- By DeepMind

Box 3: Our definition of "graph"



Here we use "graph" to mean a directed, attributed multi-graph with a global attribute. In our terminology, a node is denoted as $\mathbf{v}_i$, an edge as $\mathbf{e}_k$, and the global attributes as $\mathbf{u}$. We also use s_k and r_k to indicate the indices of the sender and receiver nodes (see below), respectively, for edge k. To be more precise, we define these terms as:

Directed : one-way edges, from a "sender" node to a "receiver" node.
Attribute : properties that can be encoded as a vector, set, or even another graph.
Attributed : edges and vertices have attributes associated with them.
Global attribute : a graph-level attribute.
Multi-graph : there can be more than one edge between vertices, including self-edges.

Figure 2 shows a variety of different types of graphs corresponding to real data that we may be interested in modeling, including physical systems, molecules, images, and text.

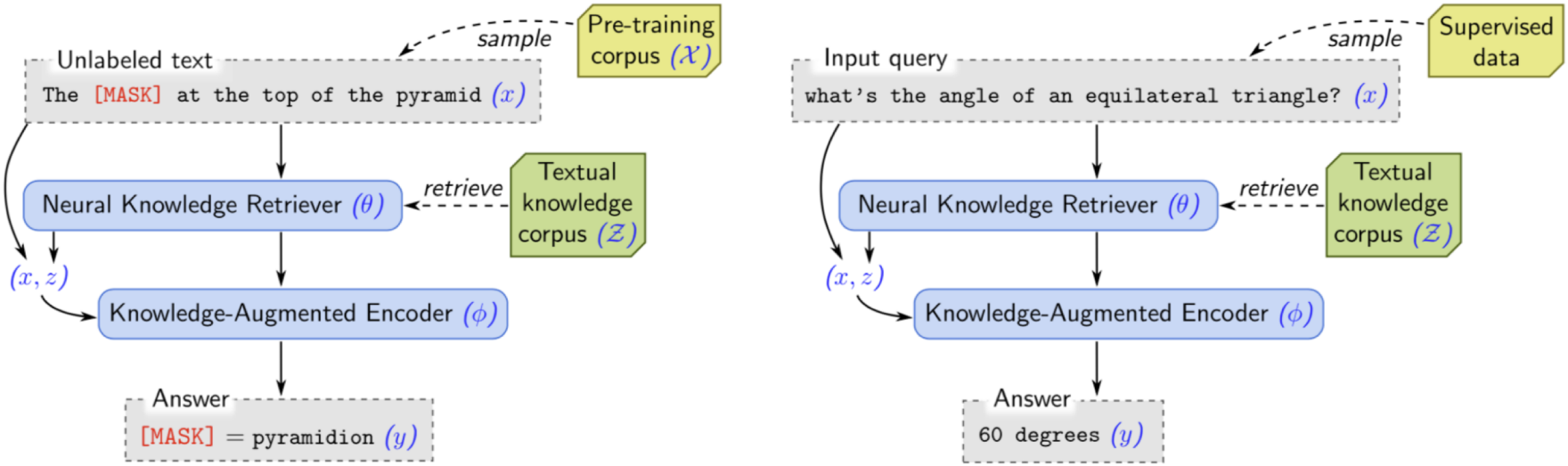
https://arxiv.org/abs/1806.01261

REALM: Retrieval-Augmented LM

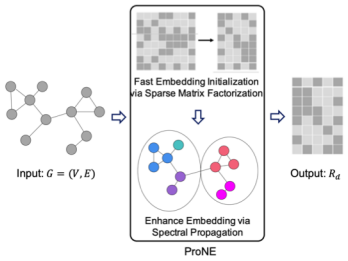
$$\text{BERT} : p(y|x)$$

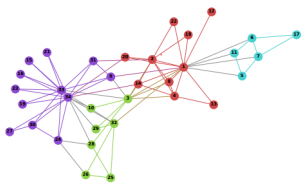
$$\text{REALM} : p(y|x) = \sum_{z \in \mathcal{Z}} p(y|z,x)p(z|x)$$

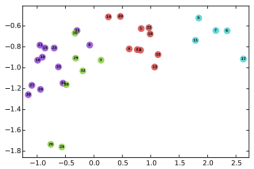
- where *Z* is the supporting set.



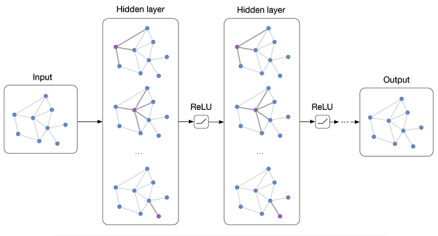
Graph Embedding&GNN: A Quick Summary

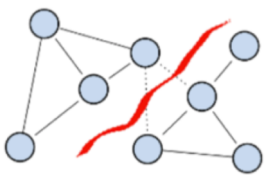






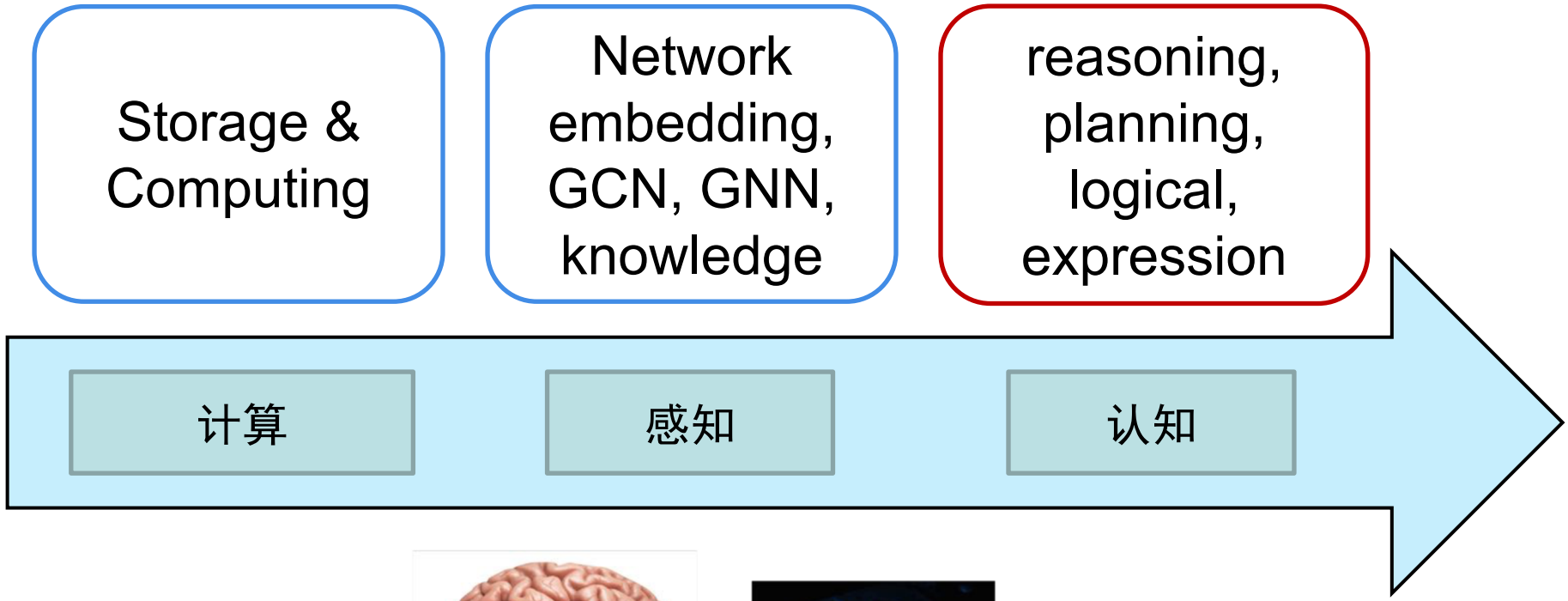
Cognitive Graph	2019: Ding et al., ACL'19
ProNE, GATNE, BurstGraph	2019: Zhang et al., IJCAI'19; Cen et al., KDD'19; Zhao et al., IJCAI'19
FastGCNs, Graph attention	2018: Velickovic et al., ICLR'18, Chen et al., ICLR 2018
NetMF & NetSMF	2018: Qiu et al., WSDM'18 & WWW'19
Neural message passing, GraphSage	2017: Gilmer et al., ICML'17; Hamilton et al., NIPS'17
Gated graph neural network	2016: Li et al., ICLR'16
structure2vec	2016: Dai et al., ICML'16
Graph convolutional network	2015: Duvenaud et al., NIPS'15; Kipf & Welling ICLR'17
PTE, metapath2vec	2015: Tang et al., KDD'15; Dong et al., KDD'17
LINE, node2vec	2015: Tang et al., WWW'15; Grover & Leskovec, KDD'16
DeepWalk	2014: Perozzi et al., KDD'14
Spectral graph convolution	2014: Bruna et al., ICLR'14
word2vec (skip-gram)	2013: Mikolov et al., ICLR'13
Graph neural network	2005: Gori et al., IJCNN'05
Spectral clustering	2000: Ng et al. & Shi, Malik
Spectral partitioning	1973: Donath & Hoffman





面向认知的GNN

- From perceptron to cognition



Stochastic vs Deterministic

Uncertainty!

Related Publications

- Ming Ding, Chang Zhou, Qibin Chen, Hongxia Yang, and Jie Tang. Cognitive Graph for Multi-Hop Reading Comprehension at Scale. ACL'19.
- Jie Zhang, Yuxiao Dong, Yan Wang, Jie Tang, and Ming Ding. ProNE: Fast and Scalable Network Representation Learning. IJCAI'19.
- Yukuo Cen, Xu Zou, Jianwei Zhang, Hongxia Yang, Jingren Zhou and Jie Tang. Representation Learning for Attributed Multiplex Heterogeneous Network. KDD'19.
- Fanjin Zhang, Xiao Liu, Jie Tang, Yuxiao Dong, Peiran Yao, Jie Zhang, Xiaotao Gu, Yan Wang, Bin Shao, Rui Li, and Kuansan Wang. OAG: Toward Linking Large-scale Heterogeneous Entity Graphs. KDD'19.
- Qibin Chen, Junyang Lin, Yichang Zhang, Hongxia Yang, Jingren Zhou and Jie Tang. Towards Knowledge-Based Personalized Product Description Generation in E-commerce. KDD'19.
- Yifeng Zhao, Xiangwei Wang, Hongxia Yang, Le Song, and Jie Tang. Large Scale Evolving Graphs with Burst Detection. IJCAI'19.
- Yu Han, Jie Tang, and Qian Chen. Network Embedding under Partial Monitoring for Evolving Networks. IJCAI'19.
- Yifeng Zhao, Xiangwei Wang, Hongxia Yang, Le Song, and Jie Tang. Large Scale Evolving Graphs with Burst Detection. IJCAI'19.
- Jiezhong Qiu, Yuxiao Dong, Hao Ma, Jian Li, Chi Wang, Kuansan Wang, and Jie Tang. NetSMF: Large-Scale Network Embedding as Sparse Matrix Factorization. WWW'19.
- Jiezhong Qiu, Jian Tang, Hao Ma, Yuxiao Dong, Kuansan Wang, and Jie Tang. DeepInf: Modeling Influence Locality in Large Social Networks. KDD'18.
- Jiezhong Qiu, Yuxiao Dong, Hao Ma, Jian Li, Kuansan Wang, and Jie Tang. Network Embedding as Matrix Factorization: Unifying DeepWalk, LINE, PTE, and node2vec. WSDM'18.
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Thank you !

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