Integrating Domain-Knowledge into Deep Learning

Russ Salakhutdinov

Machine Learning Department
rsalakhu@cs.cmu.edu

Carnegie Mellon University

MACHINE LEARNING DEPARTMENT

Impact of Deep Learning

- Speech Recognition
- Computer Vision
- Recommender Systems
- Language Understanding
- Drug Discovery and Medical Image Analysis

Domain knowledge

- Two key ingredients of a Statistical Machine Learning system
  - Model architecture/class
  - Learning algorithms to learn from data
- How do we incorporate domain knowledge into either or both these ingredients?
- We can consider three classes of domain knowledge:
  - Relational
  - Logical
  - Scientific

Relational Knowledge

- Simple relations among entities
  - (father, Bob, Alice)
- Available via relational databases, or knowledge graphs

- Statistical Relational Models
  - Probabilistic Graphical Models (PGMs) to model relationships amongst entities
  - Probabilistic Relational Models (via Bayes Nets), Relational Dependency Networks
- Embeddings
  - Instead of distributional semantics, represent entities via vectors in some vector space
  - Learn these vector representations via predicting an entity given its "context"

- We show how to incorporate relational information in Deep Learning via knowledge graph propagation

Ravikumar, Salakhutdinov, 2019

Logical Knowledge

- Propositional and First Order Logic (FOL) based knowledge
  - In contrast to simpler tuple based relational knowledge
  - E.g. if object has a wing, and a beak, it is a bird
- Encode logical knowledge into Probabilistic Graphical Models
- Bayesian Networks from Horn clauses, Probabilistic Context Free Grammars, Markov Logic Networks
- We incorporate logical information (and more general constraints) into Deep Learning via distillation (student-teacher) framework

Ravikumar, Salakhutdinov, 2019

Scientific Knowledge

- Partial and Stochastic Differential Equations
  - Newton Laws of Motion
  - Navier-Stokes fluid dynamics equations
  - ...
- Conservation laws and principles, Invariances

- Learning PDEs from data
- Regularizing dynamical system (e.g. state space models) via PDEs

Ravikumar, Salakhutdinov, 2019

Reading Comprehension

- **Context**: "...arrested Illinois governor **Rod Blagojevich** and his chief of staff John Harris on corruption charges ... included **Blogojevich** allegedly conspiring to sell or trade the senate seat left vacant by President-elect Barack Obama..."
- **Query**: President-elect Barack Obama said Tuesday he was not aware of alleged corruption by **X** who was arrested on charges of trying to sell Obama's senate seat.
- **Answer**: Rod Blagojevich

Onishi, Wang, Bansal, Gimpel, McAllester, EMNLP, 2016

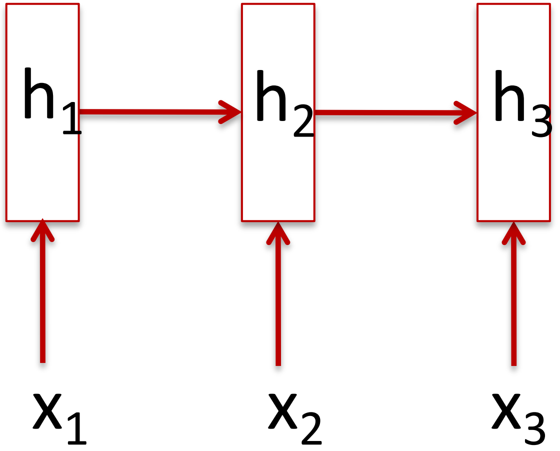
Recurrent Neural Networks (RNNs)

$$\mathbf{h_t} = \phi(\mathbf{U}\mathbf{h_{t-1}} + \mathbf{W}\mathbf{x_t} + \mathbf{b})$$

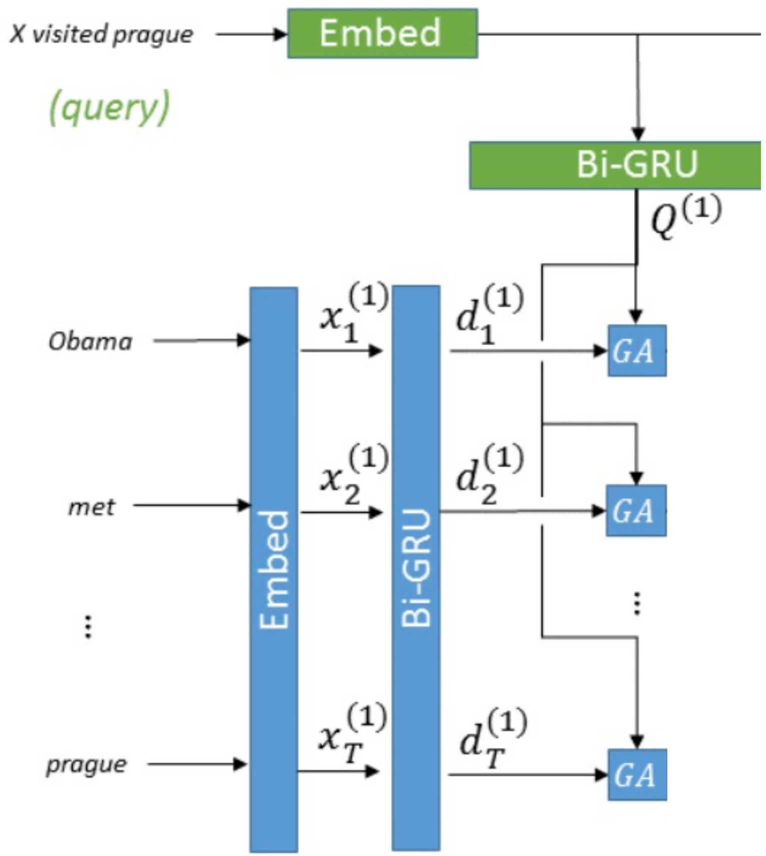
Nonlinearity

Hidden State at previous time step

Input at time step t



Gated Attention Mechanism



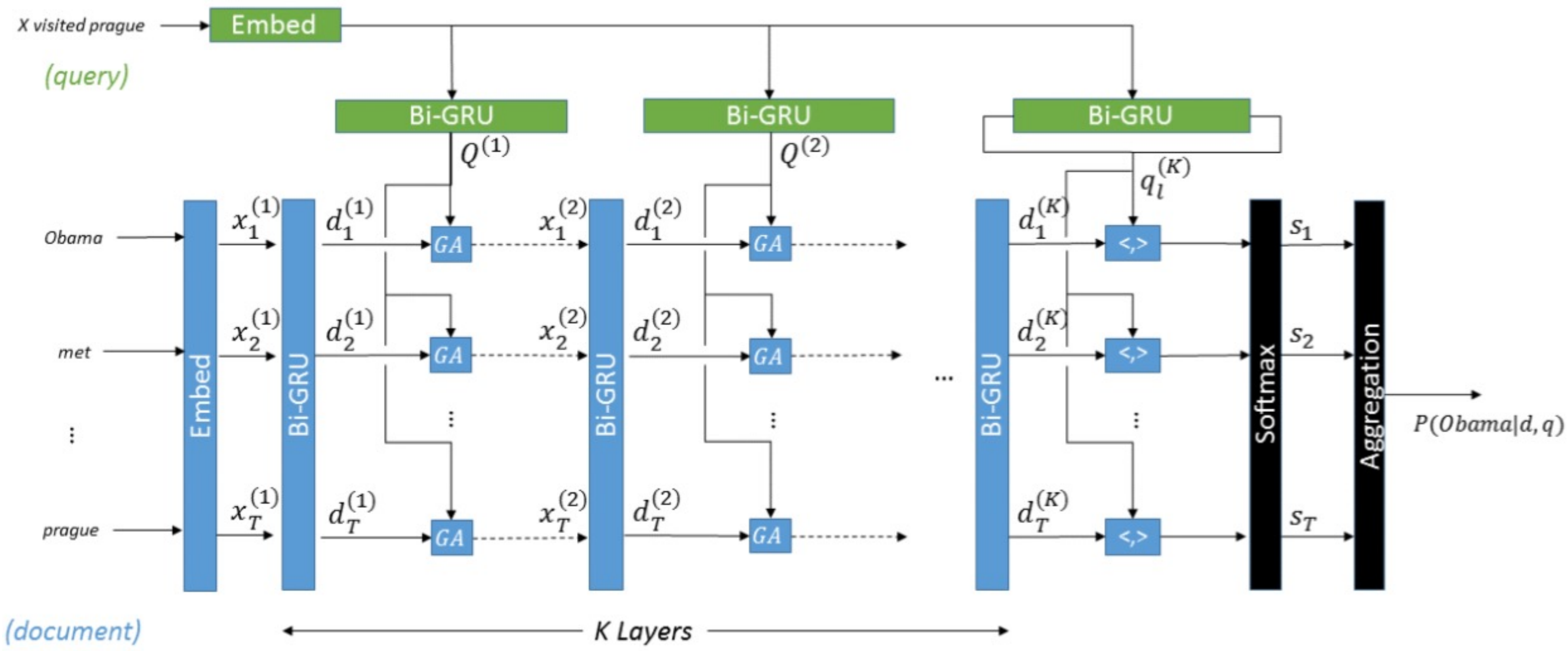
- Use Recurrent Neural Networks or Transformers to encode a document and a query.
- Use element-wise multiplication to model the interactions between document and query:

$$x_i = d_i \odot q_i$$

Dhingra, Liu, Yang, Cohen, Salakhutdinov, ACL 2017

Multi-Hop Architecture

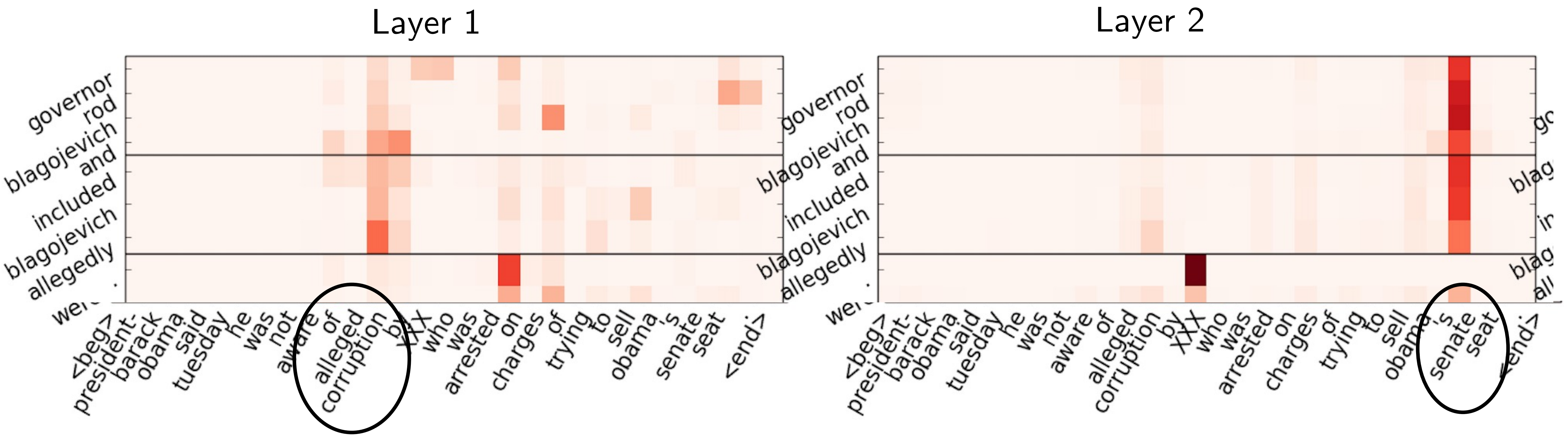
- Reasoning over multiple sentences requires several passes over the context



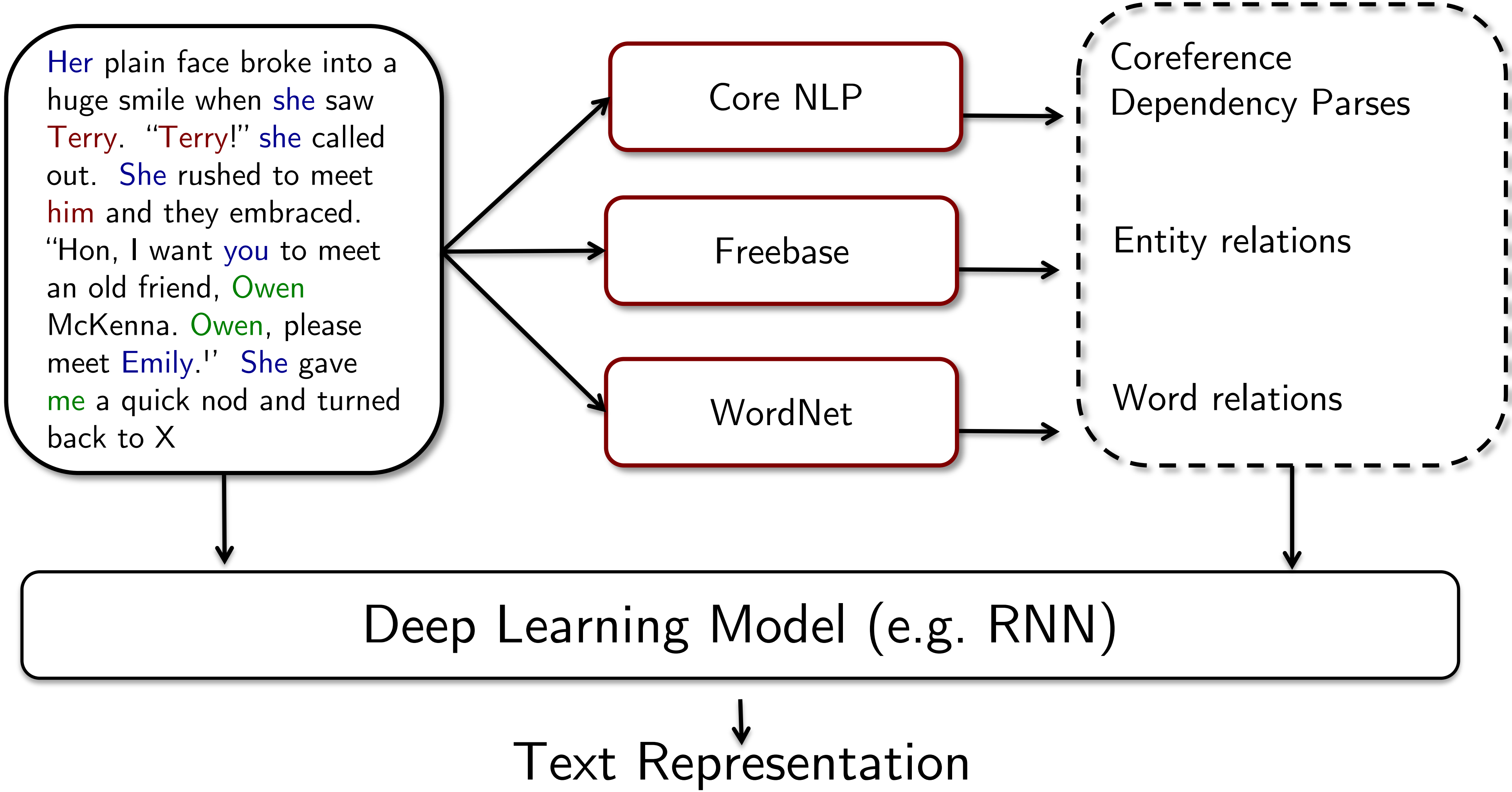
Dhingra, Liu, Yang, Cohen, Salakhutdinov, ACL 2017

Reasoning and Attention

- **Context**: "…arrested Illinois **governor Rod Blagojevich** and his chief of staff John Harris on corruption charges … **included Blogojevich** allegedly conspiring to sell or trade the **senate seat** left vacant by President-elect Barack Obama…"
- **Query**: "President-elect Barack Obama said Tuesday he was not aware of **alleged corruption** by **X** who was arrested on charges of trying to sell Obama's **senate seat**."
- **Answer**: **Rod Blagojevich**



Incorporating Prior Knowledge



Open Domain Question Answering

- Finding answers to factual questions posed in Natural Language:

Who voiced Meg in Family Guy?

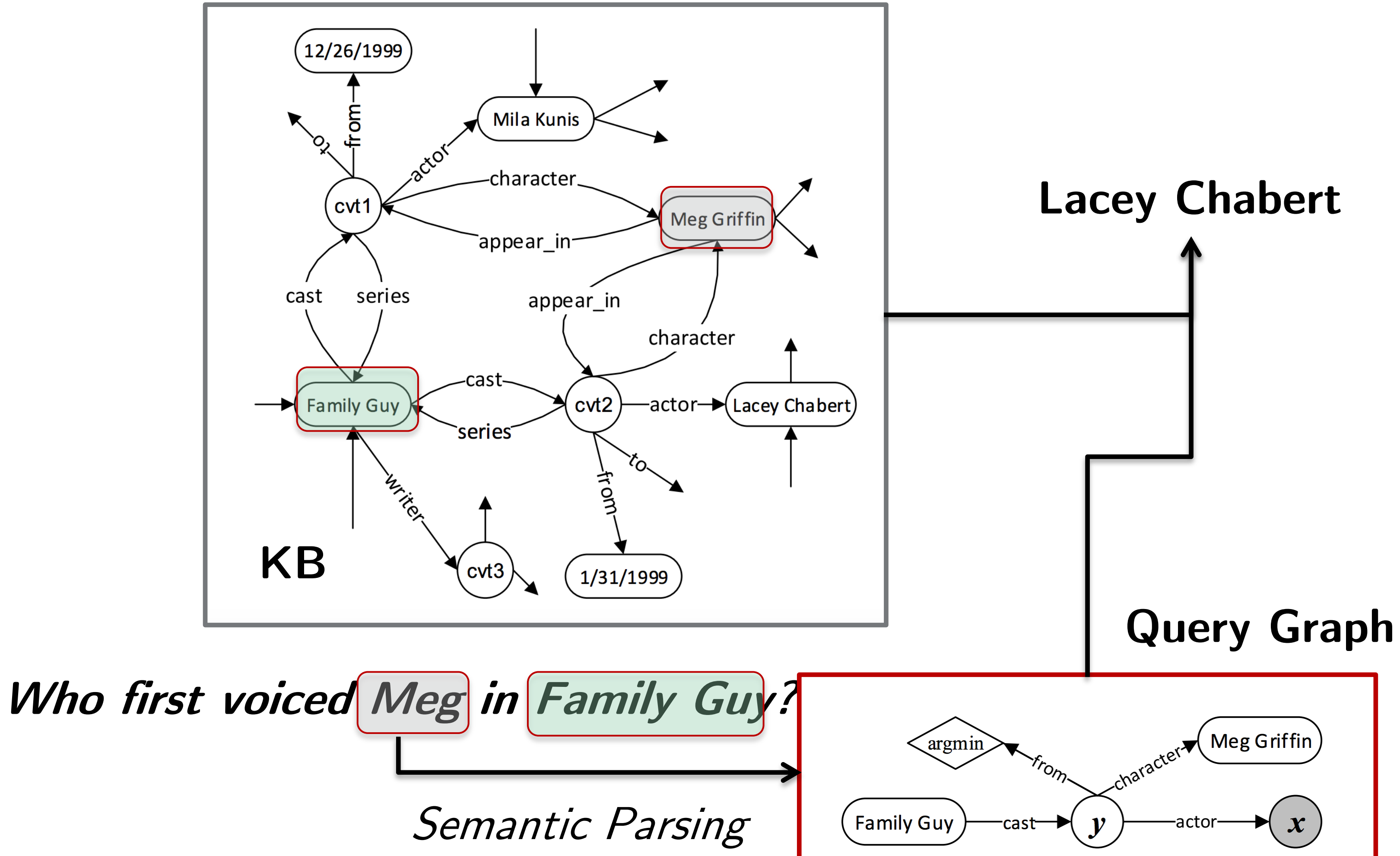
A. Lacey Chabert, Mila Kunis

Who first voiced Meg in Family Guy?

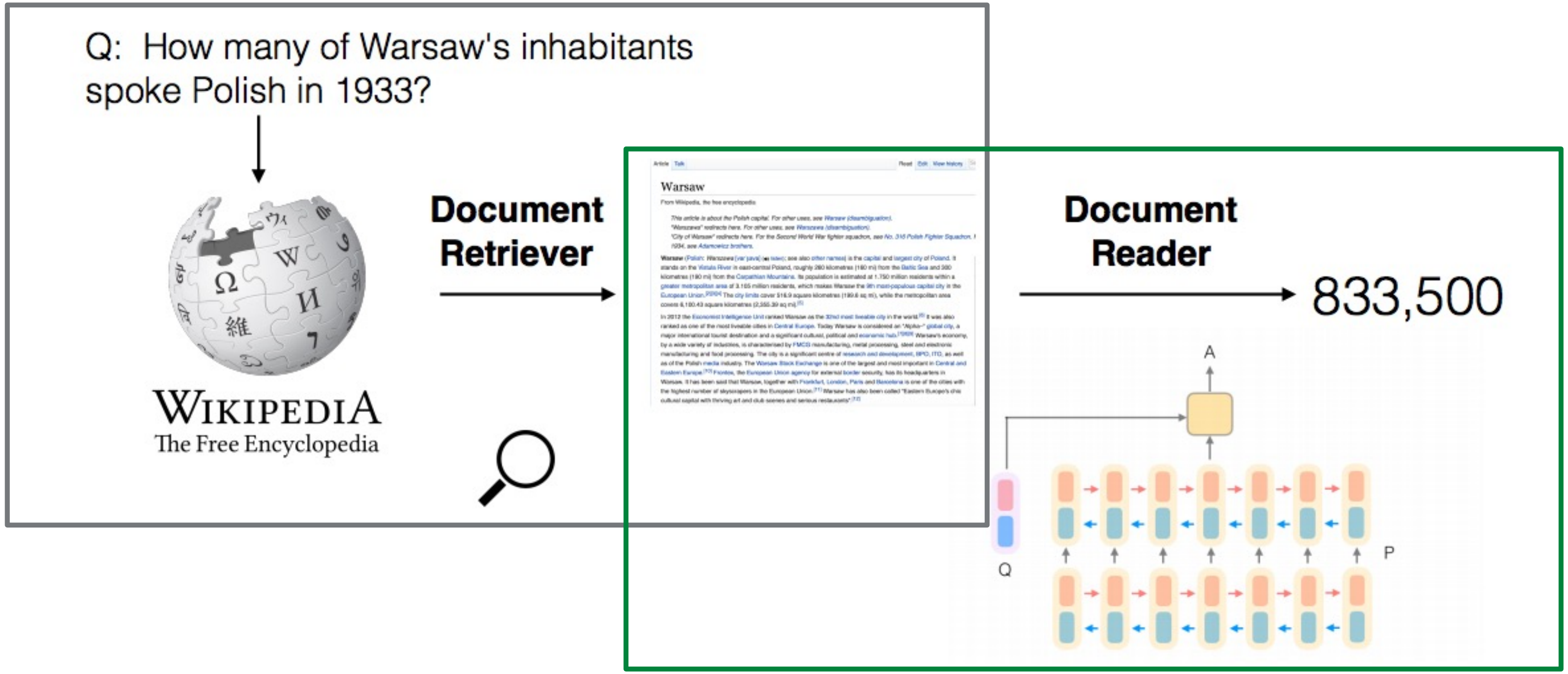
A. Lacey Chabert

Sun, Dhingra et al., EMNLP 2018

Knowledge Base as a Knowledge Source

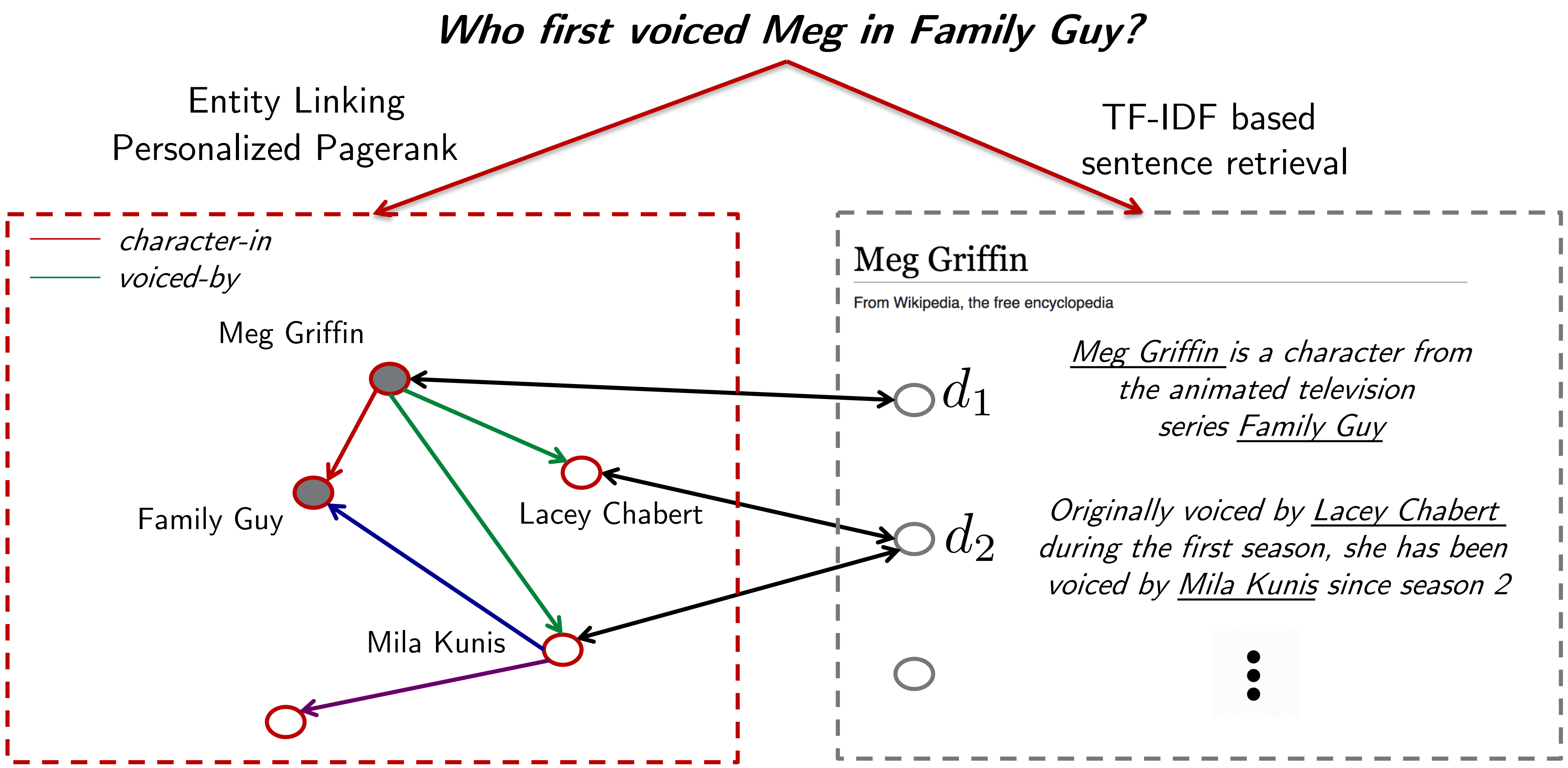


Unstructured Text as a Knowledge Source



Step 1 (Information Retrieval):
Retrieve passages relevant to the Question using shallow methods
Step 2 (Reading Comprehension):
Perform deep reading of passages to extract answers

Text Augmented Knowledge Graph (Dhingra, Sun, et al., 2018)



Dhingra, Sun, et al., EMNLP 2018

Reading Graphs

Given a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ and a natural language question $q = (w_1, \ldots, w_T)$ learn a function $y_v = f(v) \forall v \in \mathcal{V}$, s.t. $y_v \in \{0, 1\}$ and $y_v = 1$ if and only if v is an answer for q.

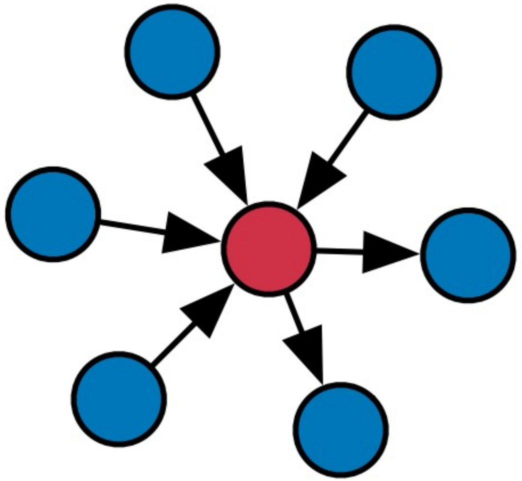
$$P(y_v = 1 | \mathcal{G}, q) = \frac{\exp h_q^T h_v}{\sum_{v'} \exp h_q^T h_{v'}}$$

h_q -- Question Representation from an LSTM

h_v -- Node Representation from a Graph Convolution Network

Dhingra, Sun, et al., EMNLP 2018

Graph Convolution Network



For each v:

Initialize $h_v^{(0)}$

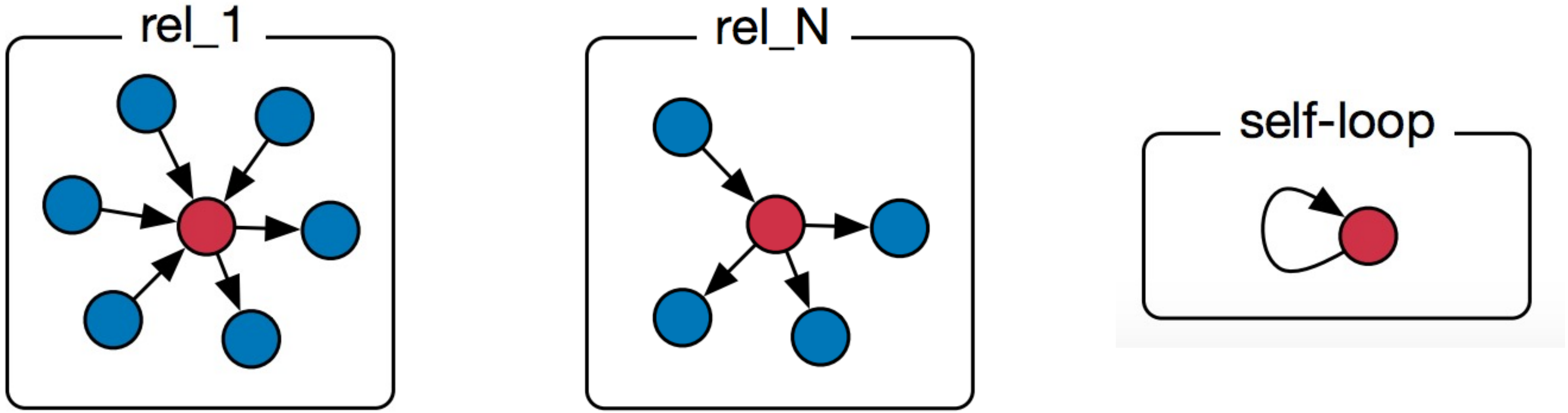
$$h_v^{(t)} = f(W_1 h_v^{(t-1)} + W_2 \sum_{v' \in N(v)} \alpha_{v'} h_{v'}^{(t-1)})$$

Repeat for $t = 1, \ldots, T$

Kipf et al., 2016

Relational Graph Convolution Network

Graphs with edge types



$$h_v^{(t)} = f\left(\sum_r W_1 h_v^{(t-1)} + W_2^r \sum_{v' \in N_r(v)} \alpha_{v'} h_{v'}^{(t-1)}\right)$$

Schlichtkrull et al. 2017

Graph Propagation / Graph Convolution

Entities

e

Meg Griffin

Lookup Table

$$h_e^{(0)} = L(e) \in \mathbb{R}^p$$

Documents

d

Meg Griffin is a character from the animated television series Family Guy

BiDirectional LSTM

$$h_d^{(0)} = \mathrm{LSTM}(d_{w_1}, \ldots, d_{w_T}) \in \mathbb{R}^{T \times p}$$

Dhingra, Sun, et al., EMNLP 2018

Graph Propagation / Graph Convolution

Entities → Documents

e → d

Meg Griffin

<u>Meg Griffin</u> is a character from the animated television series <u>Family Guy</u>

$$h_d^{(t)} = \mathrm{LSTM}(h_{d_1}^{(t-1)} || e_{w_1}^{(t-1)}, \ldots, h_{d_T}^{(t-1)} || e_{w_T}^{(t-1)})$$

---

e ← d

Meg Griffin

<u>Meg Griffin</u> is a character from the animated television series <u>Family Guy</u>

$$h_e^{(t)} = f(W_1 h_e^{(t-1)} + \sum_r \sum_{v' \in N_r(v)} W_2^r h_{v'}^{(t-1)} + W_3 \sum_{d:e \in d} h_{d_w}^{(t-1)})$$

- Relational information via KB propagation

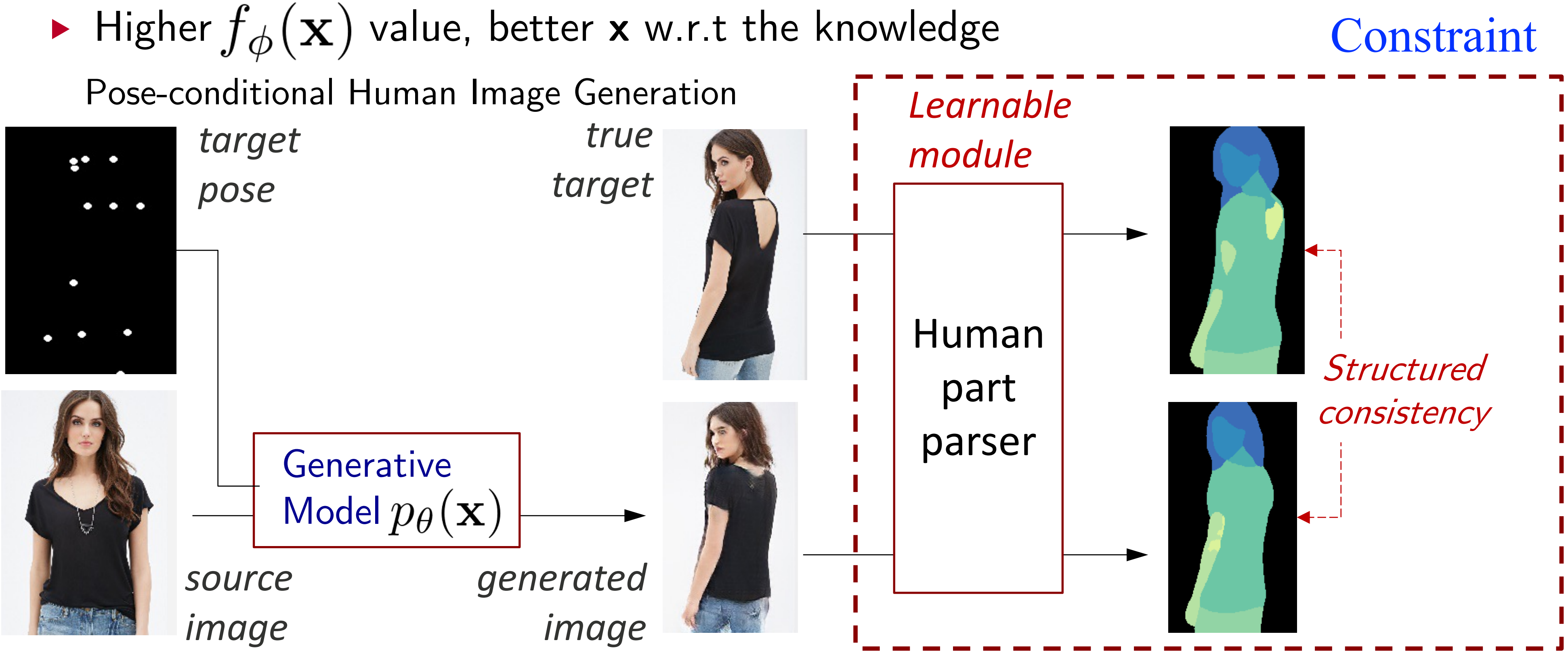
Dhingra, Sun, et al., EMNLP 2018

Domain knowledge

- We consider three classes of domain knowledge:
  - Relational
  - Logical (constraints)
  - Scientific

Learning with Constraints

- Consider a statistical model $\mathbf{x} \sim p_\theta(\mathbf{x})$
- Consider a constraint function, $f_\phi(\mathbf{x}) \in \mathbb{R}$ parameterized by ϕ
  - Higher $f_\phi(\mathbf{x})$ value, better $\mathbf{x}$ w.r.t the knowledge



DeepFashion, Liu wt al., 2016

Zhiting Hu et.al., NeurIPS 2018

Learning with Constraints

- Consider a statistical model $\mathbf{x} \sim p_\theta(\mathbf{x})$
- Consider a constraint function, $f_\phi(\mathbf{x}) \in \mathbb{R}$ parameterized by ϕ
  - Higher $f_\phi(\mathbf{x})$ value, better $\mathbf{x}$ w.r.t the knowledge

- Sentiment prediction:
  - This was a terrific movie, but the director could have done better

- Logical Rules:
  - Sentence *S* with structure *A-but-B*: => sentiment of *B* dominates

Learning with Constraints

- Consider a statistical model $\mathbf{x} \sim p_\theta(\mathbf{x})$
- Consider a constraint function, $f_\phi(\mathbf{x}) \in \mathbb{R}$ parameterized by ϕ
  - Higher $f_\phi(\mathbf{x})$ value, better **x** w.r.t the knowledge

- One way to impose the constraint is to maximize: $\mathbb{E}_{p_\theta}[f_\phi(\mathbf{x})]$
- Objective:

$$\min_\theta \left(\mathcal{L}(\theta) - \alpha \mathbb{E}_{p_\theta}[f_\phi(\mathbf{x})]\right)$$

Regular objective (e.g. cross-entropy loss, etc.)

Regularization: imposing constraints – difficult to compute

Posterior Regularization (Ganchev et al., 2010)

- Consider a statistical model $\mathbf{x} \sim p_\theta(\mathbf{x})$
- Consider a constraint function, $f_\phi(\mathbf{x}) \in \mathbb{R}$ parameterized by ϕ

$$\min_\theta \left(\mathcal{L}(\theta) - \alpha \boxed{\mathbb{E}_{p_\theta}[f_\phi(\mathbf{x})]} \right)$$

$$\mathcal{L}(\theta, q) = \underbrace{\mathrm{KL}\big(q(\mathbf{x}) || p_\theta(\mathbf{x})\big) - \lambda \mathbb{E}_q[f_\phi(\mathbf{x})]}$$

- Introduce variational distribution q, which is encouraged to stay close to p

- Objective:

$$\min_{\theta, q} \left(\mathcal{L}(\theta) + \alpha \mathcal{L}(\theta, q) \right)$$

Posterior Regularization (Ganchev et al., 2010)

$$\min_{\theta, q} \left(\mathcal{L}(\theta) + \alpha \mathcal{L}(\theta, q)\right)$$

$$\mathcal{L}(\theta, q) = \mathrm{KL}\big(q(\mathbf{x}) || p_\theta(\mathbf{x})\big) - \lambda \mathbb{E}_q\left[f_\phi(\mathbf{x})\right]$$

- Optimal solution for q:

$$q^*(\mathbf{x}) = p_\theta(\mathbf{x}) \exp\left(\lambda f_\phi(\mathbf{x})\right) / Z$$

Higher value -- higher probability under q – "soft constraint"

- How do we fit our model parameters θ ?

Logical Rule Formulation (Zhiting Hu et al., 2016)

- Consider a supervised learning: $p_\theta(y|\mathbf{x})$, e.g. deep neural network
- Input-Target space (X,Y)
- First-order logic rules: (r, λ)
  - $r(X, Y) \in [0, 1]$, could be soft
  - λ is the confidence level of the rule

- Within PR framework given l rules

$$q^*(y|\mathbf{x}) = p_\theta(y|\mathbf{x}) \exp\left(\sum_l \lambda_l r_l(y, \mathbf{x})\right)/\mathcal{Z}$$

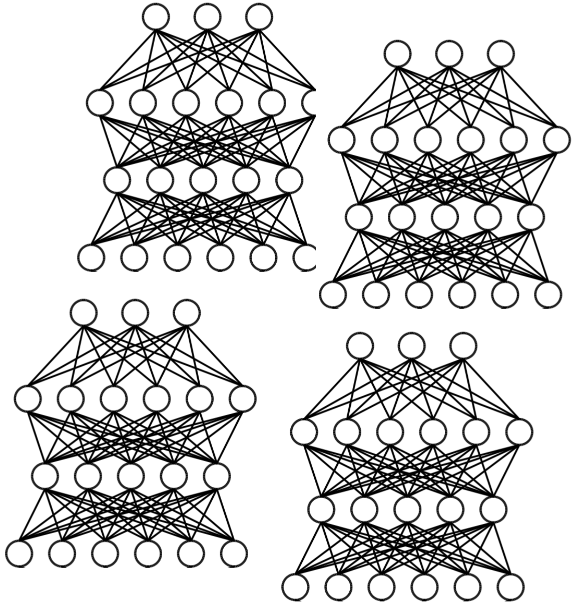
- How to train a neural network: Knowledge Distillation [Hinton et al., 2015; Bucilu et al., 2006].

Zhiting Hu et.al., ACL 2016

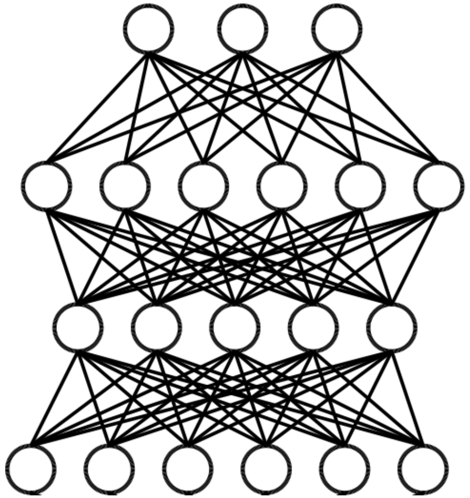
Knowledge Distillation

Match soft predictions of the teacher network and student network

$q(y|\mathbf{x})$ $\Longrightarrow$ $p_\theta(y|\mathbf{x})$



Teacher (Ensemble)



Student

Knowledge Distillation [Hinton et al., 2015; Bucilu et al., 2006].

Rule Knowledge Distillation (Zhiting Hu et al., 2016)

- Deep neural network $p_\theta(y|\mathbf{x})$
- Train to imitate the outputs of the rule-regularized teacher network
- At iteration t:

true hard label

soft prediction of $p_\theta(y|\mathbf{x})$

$$\theta^{(t+1)} = \operatorname*{argmin}_{\theta} \frac{1}{N} \sum_{n=1}^{N} \ell(y_n, \sigma_\theta(\mathbf{x})) + \alpha \ell(s_n^{(t)}, \sigma_\theta(\mathbf{x}))$$

balancing parameter

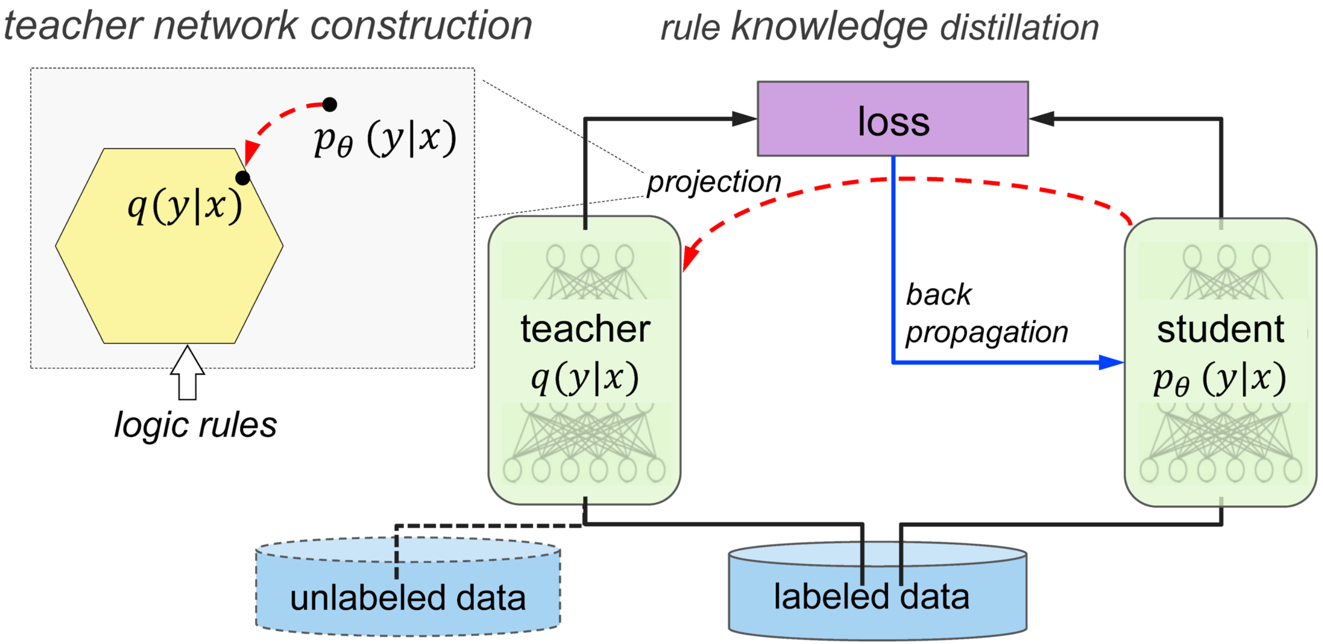
soft prediction of the teacher network q.

$$q^*(y|\mathbf{x}) = p_\theta(y|\mathbf{x}) \exp\left(\sum_l \lambda_l r_l(y, \mathbf{x})\right) / Z$$

Zhiting Hu et.al., ACL 2016

Rule Knowledge Distillation (Zhiting Hu et al., 2016)

- Deep neural network $p_\theta(y|\mathbf{x})$
- At each iteration:
  - Construct a teacher network q(y|x) with "soft constraints"
  - Train DNN to emulate the teacher network



- Sentiment classification,
- Named entity recognition

Zhiting Hu et.al., ACL 2016

Learning Rules / Constraints (Zhiting Hu et al., 2018)

$$q^*(y|\mathbf{x}) = p_\theta(y|\mathbf{x}) \exp\left(\sum_l \lambda_l r_l(y, \mathbf{x})\right) / \mathcal{Z}$$

- We can also learn the "confidence" values λ_l for logical rules

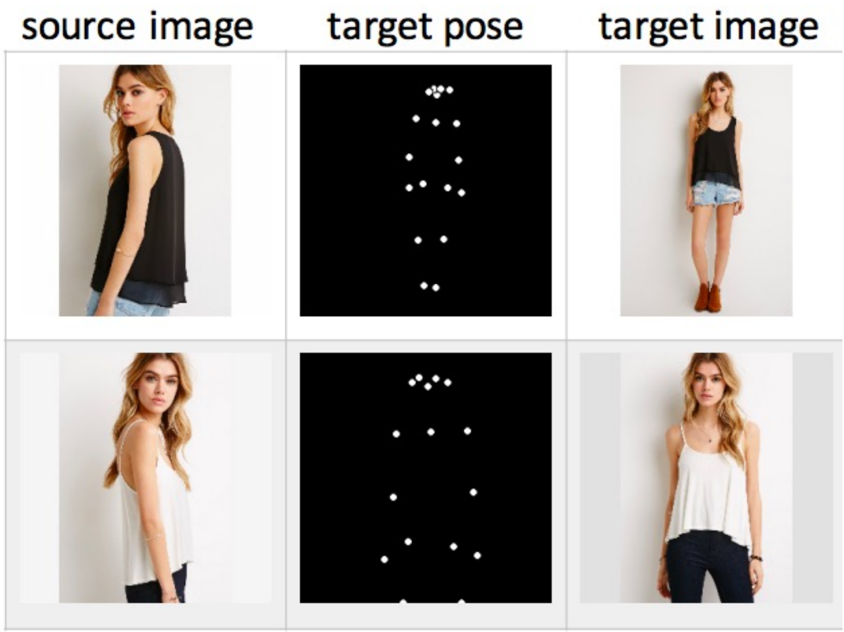
- More generally, we can optimize parameters of the constraint function $f_\phi(\mathbf{x})$

$$q^*(\mathbf{x}) = p_\theta(\mathbf{x}) \exp\left(\lambda f_\phi(\mathbf{x})\right) / \mathcal{Z}$$

  - Treat $f_\phi(\mathbf{x})$ as the reward function to be learned within the MaxEnt Inverse Reinforcement Learning

Zhiting Hu et.al., EMNLP 2016, NeurIPS2018

Pose-conditional Human Image Generation



Samples generated by the models. Enforcing learned human part constraint generates correct poses and better preserves human body structure

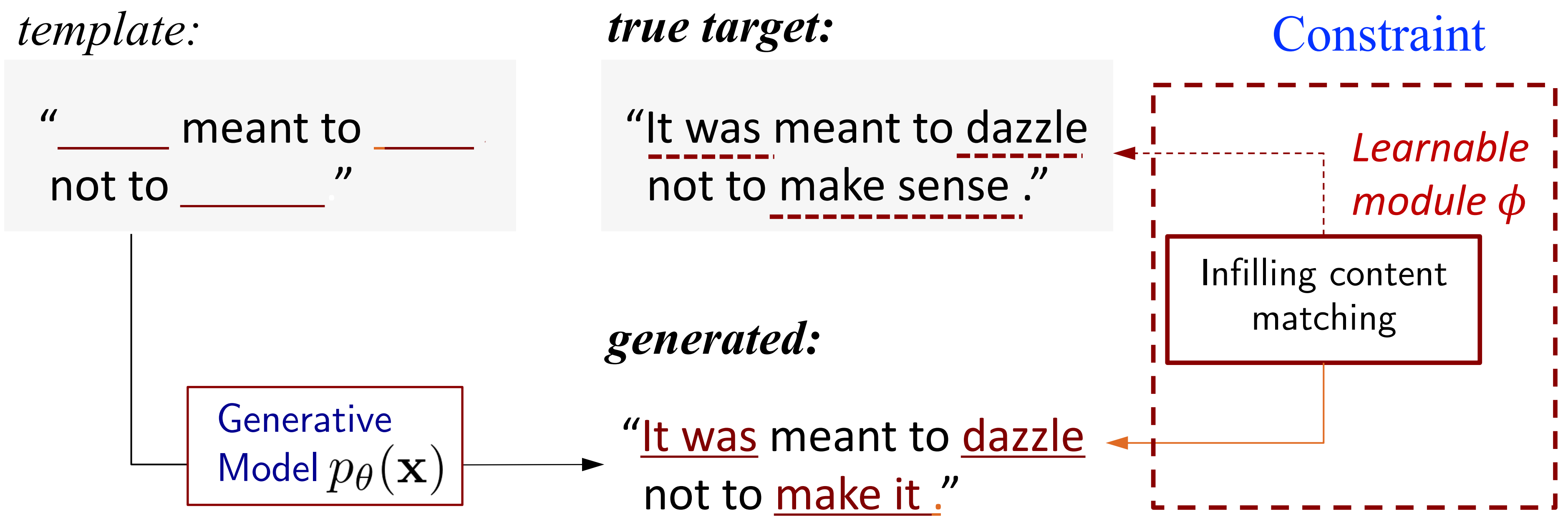
	Method	SSIM	Human
1	Ma et al. [38]	0.614	—
2	Pumarola et al. [44]	0.747	—
3	Ma et al. [37]	0.762	—
4	Base model	0.676	0.03
5	With fixed constraint	0.679	0.12
6	With learned constraint	**0.727**	**0.77**

Results of image generation using Structural Similarity (SSIM) between generated and true images

Zhiting Hu et.al., NeurIPS 2018

Template-guided Sentence Generation

- Task: Given a template, generate a complete sentence following the template
- Constraint: force to match between infilling content of the generated sentence with the true content



Zhiting Hu et.al., NeurIPS 2018

Template-guided Sentence Generation

	Model	Perplexity	Human
1	Base model	30.30	0.19
2	With binary D	30.01	0.20
3	With constraint updated in M-step (Eq.5)	31.27	0.15
4	With learned constraint	**28.69**	**0.24**

Samples by the full model are considered as of higher quality in 24% cases.

______	acting	______
the	acting	is the acting .
the	acting	is also very good .

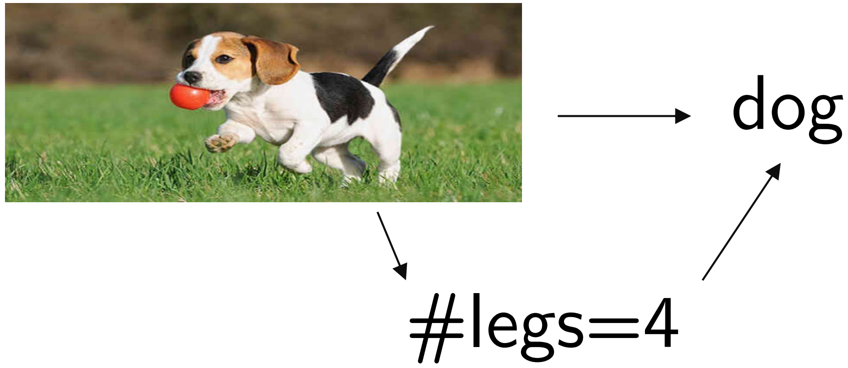
______	out of 10 .
10	out of 10 .
I will give the movie 7	out of 10 .

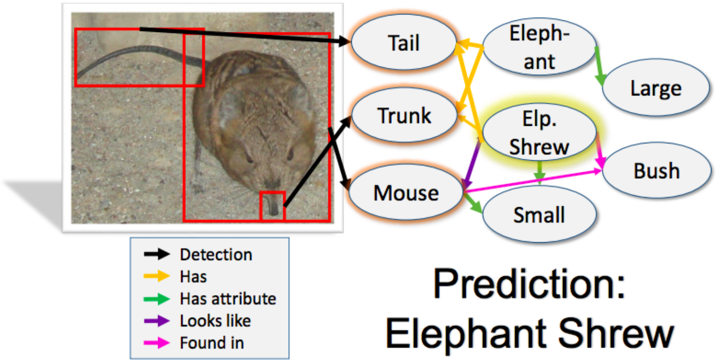
Two test examples, including the template, the sample by the base model, and the sample by the constrained model.

Zhiting Hu et.al., NeurIPS 2018

Conclusion

- Limitations: We considered very simple forms of domain knowledge: relational, logical, simple constraints
- Human Knowledge: abstract, fuzzy, build on high-level concepts
  - e.g. dogs have 4 legs





Example of how semantic knowledge about the world aids classification.

Marino et al., CVPR 2017

- How do we encode this knowledge and how do we efficiently integrate this into deep learning models