## Deep Learning for Unsupervised Relation Extraction

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LTG

Education background:

- Algorithmic, Automata Theory, Lambda Calculus...
- Machine Learning, Statistics...

Research background:

- Machine-learning-oriented NLP
- Not used to work with POS, dependency trees...
- Machine Translation, Diachronic Topic Modeling, Multimodal Semantic Role Labeling, Relation Extraction




Structuralism: interrelations are keys to our understanding of the world.


Structuralism: interrelations are keys to our understanding of the world. Realism or Nominalism - Episteme Techne
A way to abstract information for easier processing.

## Knowledge Base Population

Maps between two symbolic representations
(text and knowledge bases).
Knowledge bases are set of facts:
(entity, relation, entity)
(1) Entity
chunking
$\frac{\text { Paris }}{\downarrow}$ is the capital of France
Q90 $\longrightarrow$ P1376 $\longleftarrow$ Q142
(2) Entity
linking
(3) Relation
extraction

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## Symbolic Representations

## symbol $\leftrightarrow$ concept

e.g.: one-hot vector, text (Paris is the capital of France), knowledge base (Paris ${ }^{\text {Q90 }}$, capita $\mathrm{P}^{\mathrm{P} 1376}$, France ${ }^{\text {Q142 }}$ )

## Distributed Representations

concept $\rightarrow$ several units; unit $\rightarrow$ part of several concepts
e.g.: embeddings, neural network activations
$\underline{\text { Megrez }}_{e_{1}}^{\text {Q850779 }}$ is a star in the northern circumpolar constellation of Ursa Major ${ }_{e_{2}}^{\text {Q10460 }}$.
$\underline{\text { Posidonius }}_{e_{1}}^{\text {Q185770 }}$ was a Greek philosopher, astronomer, historian, mathematician, and teacher native to Apamea, Syria $e_{2}^{\text {Q617550 }}$.
 land of Rhodes, Greece.

In an unsupervised fashion.
Two kind of approaches: clustering and similarity function.
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Hipparchus ${ }_{e}^{\text {Q159905 }}$ was born in Nicaea, Bithynia $_{e_{2}}^{\text {Q739037 }}$, and probably died on the island of Rhodes, Greece.
$e_{1}$ part of constellation $e_{2}$
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Same cluster $\Longleftrightarrow$ Same relation
Induced clusters need not be labeled with a relation.

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$\left.\frac{\text { Megrez }_{e_{1}}^{\text {Q850779 }} \text { is a star in the northern circum- }}{\text { polar constellation of Ursa Major } \underline{e_{2}}} \underline{\text { Q10460 }}^{104}.\right\} x_{1}$
Posidonius $e_{1}^{\text {Q185770 }}$ was a Greek philosopher, astronomer, historian, mathematician, and $\left\langle x_{2}\right.$ teacher native to Apamea, Syria $e_{2}^{\text {Q617550 }}$.

Learn a similarity function $\operatorname{sim}: \mathcal{D} \times \mathcal{D} \rightarrow \mathbb{R}$

$$
\begin{aligned}
& \operatorname{sim}\left(x_{1}, x_{2}\right)<\operatorname{sim}\left(x_{2}, x_{3}\right) \\
& \operatorname{sim}\left(x_{1}, x_{3}\right)<\operatorname{sim}\left(x_{2}, x_{3}\right)
\end{aligned}
$$

Hipparchus ${ }_{1}^{\text {Q159905 }}$ was born in Nicaea, Bithynia $e_{2}^{Q 739037}$, and probably died on the is-
land of Rhodes, Greece.

5 way 1 shot: given 1 query and 5 candidates, which of the candidates is most similar to the query?
Evaluated using accuracy.

## Regularizing Discriminotive Models

```
Megrez }\mp@subsup{e}{1}{Q850779}\mathrm{ is a star in the northern circum-
polar constellation of Ursa Major Q10460.
"Posidonius }\mp@subsup{e}{1}{185770}\mathrm{ (180) wa a Greek philosopher,"
astronomer, historian, mathematician, and
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land of Rhodes, Greece.
Same cluster \(\Longleftrightarrow\) Same relation Induced clusters need not be labeled with a relation. Evaluated using clustering metrics similar to standard \(F_{1} /\) precision/recall.
```

1. Related work
2. Limitation: can't train deep classifier
3. Model details
4. Analysis of limitation
5. Proposed solution
6. Results

An LDA-like model:

$\theta_{d}$ distribution of relations in document $d$
$\mathrm{r}_{i}$ conveyed relation
$\phi_{r j}$ associate features to relations
$\mathrm{f}_{i}$ features:

1. bag of words of the infix;
2. surface form of the entities;
3. lemma words on the dependency path;
4. POS of the infix words;

Assume $\mathscr{H}_{\text {BICLIQUE }}: \forall r \in \mathcal{R}: \exists A, B \subseteq \mathcal{E}: r \bullet \breve{r}=A^{2} \wedge \breve{r} \bullet r=B^{2}$
Problem: Makes large independance assumptions.

A conditional $\beta$-VAE:

$\mathcal{L}_{\text {VAE }}(\boldsymbol{\theta}, \boldsymbol{\phi})=\mathcal{L}_{\text {reconstruction }}(\boldsymbol{\theta}, \boldsymbol{\phi})+\mathcal{L}_{\text {VAE REG }}(\boldsymbol{\phi})$
$\mathcal{L}_{\text {VAE REG }}(\boldsymbol{\phi})=\mathrm{D}_{\mathrm{KL}}(Q(\mathrm{r} \mid \mathbf{e} ; \boldsymbol{\phi}) \| \mathcal{U}(\mathcal{R}))$

Assume $\mathscr{H}_{\text {UNIFORM: }}$ : All relations occur with equal frequency.
$\forall r \in \mathcal{R}: P(r)=\frac{1}{|\mathcal{R}|}$
Assume $\mathscr{H}_{1 \rightarrow 1}$ : All relations are bijective.
$\forall r \in \mathcal{R}: r \bullet \breve{r} \cup \boldsymbol{I}=\breve{r} \bullet r \cup \boldsymbol{I}=\boldsymbol{I}$

Autoencode the entities $\mathbf{e}$ given the sentence features $\mathbf{f}$.

Problem: Still uses hand designed features.


Zeng et al. "Distant Supervision for Relation Extraction via Piecewise Convolutional Neural Networks" EMNLP 2015

## Experimental Setup

We introduced:

- 2 metrics (V-measure, ARI)
- 2 datasets (T-RExes)
$\mathrm{B}^{3}$ Similar to standard $F_{1}$
V-measure Entropic $F_{1}$
ARI Pair of samples consistency

| Model |  | $\mathrm{B}^{3}$ |  |  | V-measure |  |  | ARI |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Classifier | Reg. | $F_{1}$ | Prec. | Rec. | $F_{1}$ | Hom. | Comp. |  |
| rel-LDA |  | 29.1 | 24.8 | 35.2 | 30.0 | 26.1 | 35.1 | 13.3 |
| rel-LDA 1 |  | 36.9 | 30.4 | 47.0 | 37.4 | 31.9 | 45.1 | 24.2 |
| Linear | $\mathcal{L}_{\text {Vae reg }}$ | 35.2 | 23.8 | 67.1 | 27.0 | 18.6 | 49.6 | 18.7 |
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Yao et al. "Structured Relation Discovery using Generative Models" EMNLP 2011

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Marcheggiani and Titov "Discrete-State Variational Autoencoders for Joint Discovery and Factorization of Relations" TACL 2016

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Problem: Using a deep encoder does not work.

- We introduce a new formalism.
- The encoder and decoder are sub-models performing different tasks.
- The interaction between these two sub-models is problematic.
"The sol $\underline{e}_{1}$ was the currency of $\underline{?}_{e_{2}}$ between 1863 and 1985."
"The sol $\underline{e}_{e_{1}}$ was the currency of $\underline{?}_{e_{2}}$ between 1863 and 1985."
$e_{-i}$ missing entity, $e_{i}$ remaining entity, $s$ conveying sentence

$$
\text { for } i=1,2: \quad \overbrace{P\left(e_{-i} \mid s, e_{i}\right)}^{\text {fill-in-the-blank }}
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Assume $\mathscr{H}_{\text {BLANKABLE }}$ : The relation can be predicted from the text surrounding the two entities alone.
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Assume $\mathscr{H}_{\text {BLANKABLE }}$ : The relation can be predicted from the text surrounding the two entities alone.

1. Train a fill-in-the-blank model on an unsupervised dataset.
2. Throw away the entity predictor.
3. Use the classifier on new samples.


Hybrid (Marcheggiani and Titov 2016)

$$
\begin{aligned}
& \psi\left(e_{1}, r, e_{2}\right)=\psi_{\mathrm{SP}}\left(e_{1}, r, e_{2}\right)+\psi_{\text {RESCAL }}\left(e_{1}, r, e_{2}\right) \\
& P\left(e_{1} \mid r, e_{2}\right)=\frac{\exp \psi\left(e_{1}, r, e_{2}\right)}{\sum_{e^{\prime} \in \mathcal{E}} \exp \psi\left(e^{\prime}, r, e_{2}\right)}
\end{aligned}
$$

## Selectional Preferences

$\psi_{\mathrm{SP}}\left(e_{1}, r, e_{2}\right)=\boldsymbol{u}_{e_{1}}^{\top} \boldsymbol{a}_{r}+\boldsymbol{u}_{e_{2}}^{\top} \boldsymbol{b}_{r}$
$\boldsymbol{U} \in \mathbb{R}^{\mathcal{E} \times d}$ entity embeddings
$\boldsymbol{A}, \boldsymbol{B} \in \mathbb{R}^{\mathcal{R} \times d}$ relation embeddings

## RESCAL

$$
\psi_{\text {RESCAL }}\left(e_{1}, r, e_{2}\right)=\boldsymbol{u}_{e_{1}}^{\top} \boldsymbol{C}_{r} \boldsymbol{u}_{e_{2}}
$$

$$
\boldsymbol{U} \in \mathbb{R}^{\mathcal{E} \times d} \text { entity embeddings }
$$

$$
\boldsymbol{C} \in \mathbb{R}^{\mathcal{R} \times d \times d} \text { relation embeddings }
$$

$$
\overbrace{P\left(e_{-i} \mid s, e_{i}\right)}^{\text {fill-in-the-blank }}=\sum_{r \in \mathcal{R}} \overbrace{P(r \mid s)}^{\text {classifier }} \overbrace{P\left(e_{-i} \mid r, e_{i}\right)}^{\text {entity predictor }}
$$

$$
\begin{aligned}
\mathcal{L}_{\mathbb{E P}}(\boldsymbol{\theta}, \boldsymbol{\phi})=\underset{\substack{\left(\mathrm{s}, \mathrm{e}_{1}, \mathrm{e}_{\mathrm{e}}\right) \sim u(\mathcal{D}) \\
\mathrm{r} \sim \mathcal{P} \sim N(\mathrm{~s} ; \boldsymbol{\phi})}}{\mathbb{E}}[ & -\log \sigma\left(\psi\left(\mathrm{e}_{1}, \mathrm{r}, \mathrm{e}_{2} ; \boldsymbol{\theta}\right)\right) \\
& -\sum_{j=1}^{k} \underset{\mathrm{e}^{\prime} \sim \sim \mathcal{U}_{\mathcal{D}}(\varepsilon)}{\mathbb{E}}\left[\log \sigma\left(-\psi\left(\mathrm{e}_{1}, \mathrm{r}, \mathrm{e}^{\prime} ; \boldsymbol{\theta}\right)\right)\right] \\
& \left.-\sum_{j=1}^{k} \underset{\mathrm{e}^{\prime} \sim \sim \mathcal{U}_{\mathcal{D}}(\mathcal{E})}{\mathbb{E}}\left[\log \sigma\left(-\psi\left(\mathrm{e}^{\prime}, \mathrm{r}, \mathrm{e}_{2} ; \boldsymbol{\theta}\right)\right)\right]\right]
\end{aligned}
$$

$$
\begin{aligned}
& \begin{aligned}
\mathcal{L}_{\mathrm{EP}}(\boldsymbol{\theta}, \boldsymbol{\phi})=\frac{\mathbb{E}}{\substack{\left(\mathrm{s}, \mathrm{e}_{1}, \mathrm{e}_{2}\right) \sim \mathcal{U ( \mathcal { D } )} \\
\mathrm{r} \sim \operatorname{PCNN}(\mathrm{~s} ; \boldsymbol{\phi})}}[ & -\log \sigma\left(\psi\left(\mathrm{e}_{1}, \mathrm{r}, \mathrm{e}_{2} ; \boldsymbol{\theta}\right)\right) \\
& -\sum_{j=1}^{k} \underset{\mathrm{e}^{\prime} \sim \mathcal{U}_{\mathcal{D}}(\mathcal{E})}{\mathbb{E}}\left[\log \sigma\left(-\psi\left(\mathrm{e}_{1}, \mathrm{r}, \mathrm{e}^{\prime} ; \boldsymbol{\theta}\right)\right)\right]
\end{aligned} \\
& \left.-\sum_{j=1}^{k} \underset{\mathrm{e}^{\prime} \sim \mathcal{U}_{\mathcal{D}}(\mathcal{E})}{\mathbb{E}}\left[\log \sigma\left(-\psi\left(\mathrm{e}^{\prime}, \mathrm{r}, \mathrm{e}_{2} ; \boldsymbol{\theta}\right)\right)\right]\right]
\end{aligned}
$$

$\longrightarrow 1$. Take a sample uniformly from the dataset.

$$
\begin{aligned}
\mathcal{L}_{\mathrm{EP}}(\boldsymbol{\theta}, \boldsymbol{\phi})=\frac{\mathbb{E}}{\underset{\left(\mathrm{s}, \mathrm{e}_{1}, \mathrm{e}_{2}\right) \sim u(\mathcal{D})}{\mathrm{r} \sim \mathrm{CNN}(\mathrm{~s} ; \boldsymbol{\phi})]}} & -\log \sigma\left(\psi\left(\mathrm{e}_{1}, \mathrm{r}, \mathrm{e}_{2} ; \boldsymbol{\theta}\right)\right) \\
& -\sum_{j=1}^{k} \underset{\mathrm{e}^{\prime} \sim \mathcal{U}_{\mathcal{D}}(\mathcal{E})}{\mathbb{E}}\left[\log \sigma\left(-\psi\left(\mathrm{e}_{1}, \mathrm{r}, \mathrm{e}^{\prime} ; \boldsymbol{\theta}\right)\right)\right] \\
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\end{aligned}
$$

$\longrightarrow 1$. Take a sample uniformly from the dataset.
2. Sample a relation r from the output of the PCNN classifier.

$$
\begin{aligned}
& \begin{aligned}
\mathcal{L}_{\mathrm{EP}}(\boldsymbol{\theta}, \boldsymbol{\phi})=\underset{\substack{\left.\left(\mathbf{s}, \mathrm{e}_{1}, \mathrm{e}_{2}\right) \sim \mathcal{U}(\mathcal{D})\right]}}{\mathbb{\mathrm { r } \sim \mathcal { P C N N ( s } ; \boldsymbol { \phi } )} \mid} & {\left[-\log \sigma\left(\psi\left(\mathrm{e}_{1}, \mathrm{r}, \mathrm{e}_{2} ; \boldsymbol{\theta}\right)\right)\right.} \\
& -\sum_{j=1}^{k} \underset{\mathrm{e}^{\prime} \sim \mathcal{U}_{\mathcal{D}}(\mathcal{E})}{\mathbb{E}}\left[\log \sigma\left(-\psi\left(\mathrm{e}_{1}, \mathrm{r}, \mathrm{e}^{\prime} ; \boldsymbol{\theta}\right)\right)\right]
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\end{aligned}
$$

$\longrightarrow 1$. Take a sample uniformly from the dataset.
2. Sample a relation r from the output of the PCNN classifier.
3. Increase the energy of this fact.


Degenerate distributions


$$
\begin{align*}
& P\left(\mathrm{r} \mid s_{1}\right)=-- \\
& P\left(\mathrm{r} \mid s_{2}\right)=- \\
& P\left(\mathrm{r} \mid s_{3}\right)=- \\
& P\left(\mathrm{r} \mid s_{4}\right)=-
\end{align*}
$$

## VAE Model Reminder (Marcheggiani)

$\overbrace{P\left(e_{-i} \mid s, e_{i}\right)}^{\text {fill-in-the-blank }}=\sum_{r \in \mathcal{R}} \overbrace{P(r \mid s)}^{\text {classifier }} \overbrace{P\left(e_{-i} \mid r, e_{i}\right)}^{\text {entity predictor }}$
$\mathcal{L}_{\text {VAE REG }}(\boldsymbol{\phi})=\mathrm{D}_{\mathrm{KL}}(Q(\mathrm{r} \mid \mathbf{e} ; \boldsymbol{\phi}) \| U(\mathcal{R}))$

Degenerate distributions
$P\left(\mathrm{r} \mid s_{1}\right)=\square$
$P\left(\mathrm{r} \mid s_{2}\right)=$
$P\left(\mathrm{r} \mid s_{3}\right)=$
$P\left(\mathrm{r} \mid s_{4}\right)=$

$$
\begin{aligned}
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Problem: Marcheggiani's model cannot handle deep encoder.

Desired distribution


## VAE Model Reminder (Marcheggiani)

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$\mathcal{L}_{\text {VAE REG }}(\boldsymbol{\phi})=\mathrm{D}_{\mathrm{KL}}(Q(\mathrm{r} \mid \mathbf{e} ; \boldsymbol{\phi}) \| U(\mathcal{R}))$

Degenerate distributions:


Desired distributions:


## Ensure Confidence

$$
\mathcal{L}_{S}(\phi)=\underset{(\mathrm{s}, \mathbf{e}) \sim u(\mathcal{D})}{\mathbb{E}}[\mathrm{H}(\mathrm{R} \mid \mathrm{s}, \mathbf{e} ; \boldsymbol{\phi})]
$$

The entropy of the relation distribution must be low for each sample.

Degenerate distributions:


## Ensure Diversity

$$
\mathcal{L}_{\mathrm{D}}(\boldsymbol{\phi})=\mathrm{D}_{\mathrm{KL}}(P(\mathrm{R} \mid \boldsymbol{\phi}) \| \mathcal{U}(\mathcal{R}))
$$

Desired distributions:

$$
P\left(\mathrm{r} \mid s_{1}\right)=-\square-\square-\square
$$

$$
P\left(\mathrm{r} \mid s_{2}\right)=
$$

$$
P\left(\mathrm{r} \mid s_{3}\right)=
$$

$$
P\left(\mathrm{r} \mid s_{4}\right)=
$$

At the level of the dataset (or mini-batch) the distribution of relations must be uniform.

| Model |  | $\mathrm{B}^{3}$ |  |  | V -measure |  |  | ARI |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
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| BERTcoder | $\mathcal{L}_{S}+\mathcal{L}_{\text {D }}$ | 41.5 | 34.6 | 51.8 | 39.9 | 33.9 | 48.5 | 35.1 |
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| Linear | $\mathcal{L}_{\text {VAE REG }}$ | 35.2 | 23.8 | 67.1 | 27.0 | 18.6 | 49.6 | 18.7 |
| PCNN | $\mathcal{L}_{\text {VaE ReG }}$ | 27.6 | 24.3 | 31.9 | 24.7 | 21.2 | 29.6 | 15.7 |
| Linear | $\mathcal{L}_{S}+\mathcal{L}_{\text {D }}$ | 37.5 | 31.1 | 47.4 | 38.7 | 32.6 | 47.8 | 27.6 |
| PCNN | $\mathcal{L}_{S}+\mathcal{L}_{\text {D }}$ | 39.4 | 32.2 | 50.7 | 38.3 | 32.2 | 47.2 | 33.8 |
| BERTcoder | $\mathcal{L}_{S}+\mathcal{L}_{\text {D }}$ | 41.5 | 34.6 | 51.8 | 39.9 | 33.9 | 48.5 | 35.1 |
| BERTcoder | Selfore | 49.1 | 47.3 | 51.1 | 46.6 | 45.7 | 47.6 | 40.3 |


| Model |  | $\mathrm{B}^{3}$ |  |  | V -measure |  |  | ARI |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Classifier | Reg. | $F_{1}$ | Prec. | Rec. | $F_{1}$ | Hom. | Comp. |  |
| rel-LDA |  | 29.1 | 24.8 | 35.2 | 30.0 | 26.1 | 35.1 | 13.3 |
| rel-LDA1 |  | 36.9 | 30.4 | 47.0 | 37.4 | 31.9 | 45.1 | 24.2 |
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Hu et al. "SelfORE: Self-supervised Relational Feature Learning for Open Relation Extraction" EMNLP 2020


$01234567890123456789 \quad 01234567890123456789$

| -••••••• | - . . . - | -•••• | - - . | $e_{1}$ located in $e_{2}$ |
| :---: | :---: | :---: | :---: | :---: |
| -••••• | $\cdots \bullet \bullet . .$. | - . . - | - ••• | $e_{1}$ instance of $e_{2}$ |
| -•••••... | . | - . . . | - . - . . . | $e_{1}$ in country $e_{2}$ |
| - . . . . . - | - - | - - - | - . - . | $e_{2}$ instance of $e_{1}$ |
|  | - | -••••• | - | $e_{1}$ shares border $e_{2}$ |
|  | - . . . ••• | - - . | - | $e_{2}$ shares border $e_{1}$ |
|  | -•...... | - 0 |  | $e_{2}$ located in $e_{1}$ |
| -••••• | -•••••••• | - . - | - . . - • | $e_{2}$ in country $e_{1}$ |
|  | $\cdots \cdot \cdots \cdot{ }^{\text {- }}$ |  |  | $e_{1}$ cast member of $e_{2}$ |
| -••••••• | - •••• | $\bullet \bullet \cdot$ | $\bullet \bullet$ | $e_{2}$ capital of $e_{1}$ |
|  | - | $\bigcirc$ |  | $e_{1}$ director of $e_{2}$ |
| -•••••• | -••••• | $\cdots$. • 0 |  | $e_{1}$ has child $e_{2}$ |
| - . . . . . - | $\cdots \cdot \bullet$ • | $\ldots$. . - ${ }^{\text {- }}$ |  | $e_{2}$ has child $e_{1}$ |
| - | $\bullet$ | - . . - | - | $e_{1}$ member of $e_{2}$ |
|  | - ••• |  |  | $e_{1}$ capital of $e_{2}$ |
| Rel-LDA 1 | Linear $+\mathcal{L}_{\text {VAE }}$ REG | Linear $+\mathcal{L}_{S}+\mathcal{L}_{D}$ | $\mathrm{PCNN}+\mathcal{L}_{S}+\mathcal{L}_{D}$ |  |

## 0123456789 <br> 0123456789

0123456789
0123456789

| -••••• | - •••• | -•••• | $\bullet \bullet . . .$ | $e_{1}$ located in $e_{2}$ <br> $e_{1}$ instance of $e_{2}$ |
| :---: | :---: | :---: | :---: | :---: |
| -••• | -••• | $\bullet$ • - | - | $e_{1}$ in country $e_{2}$ |
| - | - - | - . . - . | - . . - . | $e_{2}$ instance of $e_{1}$ |
| -•••••••• | -••• | -•••• | - 0 | $e_{1}$ shares border $e_{2}$ |
|  | - . . - ••• | -•••••• | $\cdots \cdot$ | $e_{2}$ shares border $e_{1}$ |
| -••••••• | - . • . . - | - . |  | $e_{2}$ located in $e_{1}$ |
| -•••••••• | $\cdots \cdots \cdot \cdots$ | - . - | - - . - - | $e_{2}$ in country $e_{1}$ |
| $\cdots \cdot \bullet$ | - • | - |  | $e_{1}$ cast member of $e_{2}$ |
| -•••••• | -• | - • | - - | $e_{2}$ capital of $e_{1}$ |
| . . . . . ${ }^{\text {e }}$ | - | - | - | $e_{1}$ director of $e_{2}$ |
| -••••••• | - . . . • $\bullet$ | - |  | $e_{1}$ has child $e_{2}$ |
| -•••••••• | - . - 0 | - $\bullet$ | $\cdots$ | $e_{2}$ has child $e_{1}$ |
| - . . . . . . | -• . - - |  | - | $e_{1}$ member of $e_{2}$ |
|  | -••••• | - . . - |  | $e_{1}$ capital of $e_{2}$ |
| Rel-LDA1 | $\underbrace{}_{\text {Linear }+\mathcal{L}_{\text {VAE REG }}}$ | $\underbrace{}_{\text {Linear }+\mathcal{L}_{S}+\mathcal{L}_{\text {D }}}$ | $\mathrm{PCNN}+\mathcal{L}_{S}+\mathcal{L}_{\text {D }}$ |  |












## Take-home Message

Selecting good regularizations to enforce modeling hypotheses enables us to train a deep classifier.

## Contributions

- Train a PCNN without supervision
- Designed two regularization losses (Skewness, Distribution distance)
- Introduced new datasets (T-RExes)
- Evaluated using additional metrics (V-measure, ARI)


# Graph-based Aggregate Extraction 

$\left.\begin{array}{l}\text { Megrez }_{e_{1}}^{\text {Q850779 }} \text { is a star in the northern circum- } \\ \text { polar constellation of Ursa Major } \underline{e}_{2}^{\text {Q10460 }} .\end{array}\right\} x_{1}$
Posidonius $_{e_{1}}^{\text {Q185770 }}$ was a Greek philosopher, astronomer, historian, mathematician, and $\left\langle x_{2}\right.$ teacher native to Apamea, Syria $e_{2}^{\text {Q617550 }}$.

Learn a similarity function $\operatorname{sim}: \mathcal{D} \times \mathcal{D} \rightarrow \mathbb{R}$

$$
\begin{aligned}
& \operatorname{sim}\left(x_{1}, x_{2}\right)<\operatorname{sim}\left(x_{2}, x_{3}\right) \\
& \operatorname{sim}\left(x_{1}, x_{3}\right)<\operatorname{sim}\left(x_{2}, x_{3}\right)
\end{aligned}
$$



5 way 1 shot: given 1 query and 5 candidates, which of the candidates is most similar to the query?
Evaluated using accuracy.

Sentential approaches: extract sentences' relation independently $\left(\mathcal{S} \times \mathcal{E}^{2} \rightarrow \mathcal{R}\right)$ Aggregate approaches: maps a set of sentences to a set of facts ( $2^{\delta \times \mathcal{E}^{2}} \rightarrow 2^{\mathcal{E}^{2} \times \mathcal{R}}$ )

## Goal

Exploit dataset-level regularities to leverage additional information

## Plan

1. Model datasets as graphs
2. Related relation extraction work only uses linguistic similarities
3. Proof that topological information can be used
4. How topological features are usually extracted (GCN)
5. How to extract them differently (WL isomorphism test)
6. Experimental results
7. Perspective

## BERTcoder (linguistic)



## BERTcoder (linguistic)



## Prediction

Compare samples using:
$\operatorname{sim}\left(x, x^{\prime}\right)=\operatorname{sigmoid}($
BERTcoder $(x)^{\top}$ BERTcoder $\left.\left(x^{\prime}\right)\right)$

## BERTcoder (linguistic)



## Prediction

Compare samples using:
$\operatorname{sim}\left(x, x^{\prime}\right)=\operatorname{sigmoid}($
BERTcoder $(x)^{\top}$ BERTcoder $\left.\left(x^{\prime}\right)\right)$

Hypotheses


The exterior and interior of Freemasons' Hall continued to be a stand-in for Thames


Golitsyn's claims about Wilson were believed in particular by the senior M15 ${\underline{e_{1}}}$ counterintelligence $e_{2}$ officer Peter Wright.

In its counter-espionage $e_{2}$ and counter-intelligence roles, SMERSH $_{e_{1}}$ appears to have been extremely successful throughout World War II.

The Freemasons' Hall in London served as the filming location for Thames House $e_{1}$, the headquarters for $\underline{M I 5}_{e_{2}}$



## Proposition

Given the path $\mathrm{e}_{1} \xrightarrow{\mathrm{r}_{1}} \mathrm{e}_{2} \xrightarrow{\mathrm{r}_{2}} \mathrm{e}_{3} \xrightarrow{\mathrm{r}_{3}} \mathrm{e}_{4}$, we expect $\mathrm{r}_{1} \not \Perp \mathrm{r}_{2} \not \not \mathrm{r}_{3}$.

## Goal

Compute the mutual information $\mathrm{I}\left(\mathrm{r}_{2} ; \mathrm{r}_{1}, \mathrm{r}_{3}\right)$

## Proposition

Given the path $\mathrm{e}_{1} \xrightarrow{\mathrm{r}_{1}} \mathrm{e}_{2} \xrightarrow{\mathrm{r}_{2}} \mathrm{e}_{3} \xrightarrow{\mathrm{r}_{3}} \mathrm{e}_{4}$, we expect $\mathrm{r}_{1} \not \Perp \mathrm{r}_{2} \nVdash \mathrm{r}_{3}$.

## Goal

Compute the mutual information $\mathrm{I}\left(\mathrm{r}_{2} ; \mathrm{r}_{1}, \mathrm{r}_{3}\right)$

## Path Counting Algorithm

We can (slowly) sample walks using power of the adjacency matrix.

1. Sample a walk by chaining neighbors
2. Reject non-path
3. Count the accepted paths weighted by importance

## Path Frequency

| Frequency | Relation Surface forms | Relation Identifiers |
| :--- | :---: | :---: |
| $31.696 \%$ | country $\bullet$ diplomatic relation $\bullet \overline{\text { citizen of }}$ | $\mathrm{P} 17 \bullet \mathrm{P} 530 \bullet \overline{\mathrm{P} 27}$ |

Example of path:
Vat Phou $\xrightarrow{\text { Vat Phou }} e_{1}$ is a ruined Khmer.......the historical relationship between.... Söseki $^{\text {Sap }}$ was a Japanese $e_{2}$ novelist Natsume Sōseki

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Example of path:
Vat Phou $e_{1}$ is a ruined Khmer... ...the historical relationship between... Söseki $e_{1}$ was a Japanese $e_{2}$ novelist
Vat Phou $\longrightarrow$ Laos Japan $\xrightarrow{ } \xrightarrow{4}$ Natsume Sōseki

## Summary Statistics

$$
\begin{array}{cc}
\mathrm{I}\left(\mathrm{r}_{2} ; \mathrm{r}_{1}, \mathrm{r}_{3}\right)=\underset{r_{1}, r_{3}}{\mathbb{E}}\left[\mathrm{H}_{P\left(\mathrm{r}_{2}\right)}\left(\mathrm{r}_{2} \mid r_{1}, r_{3}\right)\right]-\mathrm{H}\left(\mathrm{r}_{2} \mid \mathrm{r}_{1}, \mathrm{r}_{3}\right) \\
2 \geqslant \\
6.95 \text { bits } & 8.01 \text { bits }
\end{array}
$$

## Modeling Hypothesis

$\mathscr{H}_{1 \text {-NeIGHBORHOOD }}:$ Two samples with the same neighborhood in the relation extraction graph convey the same relation.
$\forall a, a^{\prime} \in \mathcal{A}: \mathcal{N}(a)=\mathcal{N}\left(a^{\prime}\right) \Longrightarrow \rho(a)=\rho\left(a^{\prime}\right)$

Graph Convolutional Network


## Graph Isomorphism




## Compare Topological Features

Skip recoloring, directly compare neighborhoods in $\mathbb{R}^{d}$ :
$S(x, k)=$ samples at distance $k$ of $x$
$\mathfrak{S}(x, k)=$
$\left\{\operatorname{BERTcoder}(y) \in \mathbb{R}^{d} \mid y \in S(x, k)\right\}$

$$
W_{1}\left(\mathfrak{S}(x, 1), \mathfrak{S}\left(x^{\prime}, 1\right)\right)
$$

algorithm WEISFEILER-LEMAN
Inputs: $G=(V, E)$ graph $k$ dimensionality
Output: $\chi_{\infty}$ coloring of $k$-tuples
$\chi_{0}(\boldsymbol{x}) \leftarrow \operatorname{iso}(\boldsymbol{x}) \quad \forall \boldsymbol{x} \in V^{k}$
for $\ell=1,2, \ldots$ do
$\mathfrak{I}_{\ell} \leftarrow$ new color index
for all $\boldsymbol{x} \in V^{k}$ do $c_{\ell}(\boldsymbol{x})$ 万 $\left\{\left\{\chi_{\ell-1}(\boldsymbol{y}) \mid \boldsymbol{y} \in N^{k}(\boldsymbol{x})\right\}\right\}$ $\chi_{\ell}(\boldsymbol{x})$ т $\left(\chi_{\ell-1}(\boldsymbol{x}), c_{\ell}(\boldsymbol{x})\right)$ in $\Im_{\ell}$
until $\chi_{\ell}=\chi_{\ell-1}$ output $\chi_{\ell}$

## Redefining similarity

We keep the linguistic similarity from MTB:

$$
\operatorname{sim}_{\text {ling }}\left(x, x^{\prime}\right)=\operatorname{sigmoid}\left(\operatorname{BERTcoder}(x)^{\top} \operatorname{BERTcoder}\left(x^{\prime}\right)\right)
$$

But also define a topological similarity:
Either using GCN:

$$
\operatorname{sim}_{\text {topo }}^{\mathrm{GCN}}\left(x, x^{\prime}\right)=\operatorname{sigmoid}\left(\operatorname{GCN}(G)_{x}^{\top} \mathrm{GCN}(G)_{x^{\prime}}\right)
$$

Or 1-Wasserstein:

$$
\operatorname{sim}_{\text {topo }}^{W_{1}}\left(x, x^{\prime}\right)=-W_{1}\left(\mathfrak{S}(x, 1), \mathfrak{S}\left(x^{\prime}, 1\right)\right)
$$

Define the topolinguistic similarity as:

$$
\operatorname{sim}_{\text {topoling }}\left(x, x^{\prime}\right)=\operatorname{sim}_{\text {ling }}\left(x, x^{\prime}\right)+\lambda \operatorname{sim}_{\text {topo }}\left(x, x^{\prime}\right)
$$

| Model | Accuracy |
| :--- | :---: |
| Pre-trained |  |
| Linguistic (BERT) | 69.46 |
| Topological $\left(W_{1}\right)$ | 65.75 |
| Topolinguistic | 72.18 |
| Fine-tuned |  |
| MTB | 78.83 |
| MTB GCN-Chebyshev | 76.10 |

## Few-Shot Evaluation

1 query
5 candidates
Which candidate conveys the same relation as the query?
Random model score 20\% accuracy.

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Soares et al. "Matching the Blanks: Distributional Similarity for Relation Learning" ACL 2019

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| :--- | ---: |
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## Few-Shot Evaluation

1 query
5 candidates
Which candidate conveys the same relation as the query?
Random model score 20\% accuracy.

## Take-home Message

Topological information can be leverage for unsupervised relation extraction.

## Contributions

- Explicitly modeled the aggregate setup for the unsupervised problem.
- Provided proof on the quality of topological information.
- Proposed an approach to exploit the mutual information between topological and linguistic features.

Several directions still need to be explored.

Use the topological features to identify the relational information in the linguistic features.

$$
\mathcal{L}_{\mathrm{LT}}\left(x_{1}, x_{2}, x_{3}\right)=\max \left(\begin{array}{r}
0, \zeta+2\left(\operatorname{sim}_{\text {ling }}\left(x_{1}, x_{2}\right)-\operatorname{sim}_{\text {topo }}\left(x_{1}, x_{2}\right)\right)^{2} \\
-\left(\operatorname{sim}_{\text {ling }}\left(x_{1}, x_{2}\right)-\operatorname{sim}_{\text {lopo }}\left(x_{1}, x_{3}\right)\right)^{2} \\
-\left(\operatorname{sim}_{\text {ling }}\left(x_{1}, x_{3}\right)-\operatorname{sim}_{\text {lopo }}\left(x_{1}, x_{2}\right)\right)^{2}
\end{array}\right)
$$

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\end{array}\right)
$$

- Idealy we want to align the two similarities.

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- Idealy we want to align the two similarities.
- However to stabilize the loss we need to use negative samples.

Use the topological features to identify the relational information in the linguistic features.

$$
\mathcal{L}_{\mathrm{LT}}\left(x_{1}, x_{2}, x_{3}\right)=\max \left(\begin{array}{r}
0, \sqrt{\zeta}+2\left(\operatorname{sim}_{\text {ling }}\left(x_{1}, x_{2}\right)-\operatorname{sim}_{\text {topo }}\left(x_{1}, x_{2}\right)\right)^{2} \\
-\left(\operatorname{sim}_{\text {ling }}\left(x_{1}, x_{2}\right)-\operatorname{sim}_{\mathrm{topo}}\left(x_{1}, x_{3}\right)\right)^{2} \\
-\left(\operatorname{sim}_{\text {ling }}\left(x_{1}, x_{3}\right)-\operatorname{sim}_{\text {topo }}\left(x_{1}, x_{2}\right)\right)^{2}
\end{array}\right)
$$

- Idealy we want to align the two similarities.
- However to stabilize the loss we need to use negative samples.
- Up to a margin $\zeta$.

Questions?

## Supplementary Material

## $\mathscr{H}_{\text {DISTANT }}$

A sentence conveys all the possible relations between all the entities it contains.
$\mathcal{D}_{\mathcal{R}}=\mathcal{D} \bowtie \mathcal{D}_{\mathrm{KB}}$
where $\bowtie$ denotes the natural join operator:

$$
\mathcal{D} \bowtie \mathcal{D}_{\mathrm{KB}}=\left\{\left(s, e_{1}, e_{2}, r\right) \mid\left(s, e_{1}, e_{2}\right) \in \mathcal{D} \wedge\left(e_{1}, e_{2}, r\right) \in \mathcal{D}_{\mathrm{KB}}\right\} .
$$

1. the bag of words of the infix;
2. the surface form of the entities;
3. the lemma words on the dependency path;
4. the POS of the infix words;
5. the type of the entity pair (e.g. person-location);
6. the type of the head entity (e.g. person);
7. the type of the tail entity (e.g. location);
8. the words on the dependency path between the two entities.

$$
\begin{aligned}
\mathrm{B}^{3} \operatorname{precision}(g, c) & =\underset{\mathrm{X}, \mathrm{Y} \sim \mathcal{U}\left(\mathcal{D}_{\mathcal{R}}\right)}{\mathbb{E}} P(g(\mathrm{X})=g(\mathrm{Y}) \mid c(\mathrm{X})=c(\mathrm{Y})) \\
\mathrm{B}^{3} \operatorname{recall}(g, c) & =\underset{\mathrm{X}, \mathrm{Y} \sim \mathcal{U}\left(\mathcal{D}_{\mathfrak{R})}\right.}{ } P(c(\mathrm{X})=c(\mathrm{Y}) \mid g(\mathrm{X})=g(\mathrm{Y})) \\
\mathrm{B}^{3} F_{1}(g, c) & =\frac{2}{\mathrm{~B}^{3} \operatorname{precision}(g, c)^{-1}+\mathrm{B}^{3} \operatorname{recall}(g, c)^{-1}}
\end{aligned}
$$

$$
\begin{aligned}
\operatorname{homogeneity}(g, c) & =1-\frac{\mathrm{H}(c(\mathrm{X}) \mid g(\mathrm{X}))}{\mathrm{H}(c(\mathrm{X}))} \\
\text { completeness }(g, c) & =1-\frac{\mathrm{H}(g(\mathrm{X}) \mid c(\mathrm{X}))}{\mathrm{H}(g(\mathrm{X}))} \\
\text { V-measure }(g, c) & =\frac{2}{\operatorname{homogeneity}(g, c)^{-1}+\operatorname{completeness}(g, c)^{-1}}
\end{aligned}
$$

$$
\begin{gathered}
\mathrm{RI}(g, c)=\underset{\mathrm{X}, \mathrm{Y}}{\mathbb{E}}[P(c(\mathrm{X})=c(\mathrm{Y}) \Leftrightarrow g(\mathrm{X})=g(\mathrm{Y}))] \\
\operatorname{ARI}(g, c)=\frac{\operatorname{RI}(g, c)-\underset{c \sim u\left\langle\left(\mathcal{R}^{\mathcal{D}}\right)\right.}{\mathbb{E}}[\mathrm{RI}(g, c)]}{\max _{c \in \mathcal{R}^{\mathcal{D}}}^{\mathbb{E}} \mathrm{RI}(g, c)-\underset{c \sim u\left(\mathcal{R}^{\mathcal{D}}\right)}{\mathbb{E}}[\mathrm{Rl}(g, c)]}
\end{gathered}
$$

$$
\pi_{r}=\frac{\left(\exp \left(y_{r}\right)+\mathrm{G}_{r}\right) / \tau}{\sum_{r^{\prime} \in \mathcal{R}}\left(\exp \left(y_{r^{\prime}}\right)+\mathrm{G}_{r^{\prime}}\right) / \tau}
$$

| Confidence | $\mathrm{B}^{3}$ |  |  |  |  | V-measure |  |  |  |
| :---: | ---: | :---: | :---: | :--- | :--- | :--- | :--- | :--- | :--- |
|  | $F_{1}$ | Prec. | Rec. |  | $F_{1}$ | Hom. | Comp. |  |  |
| $\mathcal{L}_{\text {S }}$ regularization | 39.4 | 32.2 | 50.7 |  | 38.3 | 32.2 | 47.2 | 33.8 |  |
| Gumbel-Softmax | 35.0 | 29.9 | 42.2 |  | 33.2 | 28.3 | 40.2 | 25.1 |  |

$$
P(\mathrm{r}=r \mid s, \boldsymbol{e} ; \boldsymbol{\theta}, \boldsymbol{\phi})=P\left(\mathrm{r}_{s}=r \mid s ; \boldsymbol{\phi}\right) P\left(\mathrm{r}_{e}=r \mid \boldsymbol{e} ; \boldsymbol{\theta}\right)
$$

$$
\mathcal{L}_{\mathrm{ALIGN}}(\boldsymbol{\theta}, \boldsymbol{\phi})=-\log \sum_{r \in \mathcal{R}} P(r \mid s, \boldsymbol{e} ; \boldsymbol{\theta}, \boldsymbol{\phi})+\mathcal{L}_{\mathrm{D}}(\boldsymbol{\theta})+\mathcal{L}_{\mathrm{D}}(\boldsymbol{\phi}) .
$$

| Model | $\mathrm{B}^{3}$ |  |  |  |  | V-measure |  |  |  |
| :---: | ---: | :---: | :---: | :--- | :--- | :--- | :--- | :--- | :--- |
|  | $F_{1}$ | Prec. | Rec. |  | $F_{1}$ | Hom. | Comp. |  |  |
| $\mathcal{L}_{\text {EP }}+\mathcal{L}_{\mathrm{S}}+\mathcal{L}_{\mathrm{D}}$ | 39.4 | 32.2 | 50.7 |  | 38.3 | 32.2 | 47.2 | 33.8 |  |
| $\mathcal{L}_{\text {ALIGN }}$ average | 37.6 | 30.3 | 49.7 |  | 39.4 | 33.1 | 48.8 | 20.3 |  |
| $\mathcal{L}_{\text {ALIGN }}$ maximum | 41.2 | 33.6 | 53.4 |  | 43.5 | 36.9 | 53.1 | 29.5 |  |
| $\mathcal{L}_{\text {ALIGN }}$ minimum | 34.5 | 26.5 | 49.3 |  | 35.9 | 29.6 | 45.7 | 15.3 |  |

Spectral (convolution is multiplication in Fourier space)
Graph

## Euclidean

| Laplacian | $\boldsymbol{L}=\boldsymbol{D}-\boldsymbol{M}$ | $\nabla^{2}$ |
| :--- | :--- | :--- |
| ¢ Eigenfunctions | $\boldsymbol{U}$ s.t. $\boldsymbol{L}=\boldsymbol{U} \boldsymbol{\Lambda} \boldsymbol{U}^{-1}$ | $\xi \mapsto e^{2 \pi i \xi x}$ |
| Fourier transform | $\boldsymbol{U}^{\top} \boldsymbol{f}$ | $\mathscr{F}(f)=\int_{-\infty}^{\infty} f(x) e^{2 \pi i \xi x} \mathrm{~d} x$ |
| Convolution | $\boldsymbol{U}\left(\boldsymbol{U}^{\top} \boldsymbol{w} \boldsymbol{U}^{\top} \boldsymbol{f}\right)$ | $\mathscr{F}^{-1}(\mathscr{F}(w) \mathscr{F}(f))$ |

Spatial

$$
\operatorname{GCN}(\boldsymbol{X} ; \boldsymbol{W})_{v}=\operatorname{ReLU}\left(\frac{1}{|N(v)|} \sum_{n_{i} \in N(v)} \boldsymbol{W} \boldsymbol{X}_{n_{i}}\right)
$$




