# Knowledge Graphs and Natural Language Processing (KG&NLP): a symbiosis

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4th Workshop on NLP4AI





- Knowledge Graphs
- Knowledge Graphs for NLP
- Scientific Knowledge Graphs
- NLP for Knowledge Graphs
- Use Cases  $\bullet$
- Future Work

## Agenda



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# **Knowledge Graphs for NLP**

- Knowledge graphs capture knowledge about
  - Entities
  - Relations
  - Facts
  - Broader Contexts
- NLU is a knowledge-intense task (although nowadays) we are ignoring this!)
- KGs help to link a symbol in text to a `representation' of the real entity, that is a proxy of its denotation, introducing additional context



Jack "Jacky" Miller is an English soccer player born 15 December 1977 in Scunthorpe, now residing in Berlin. He began his soccer career as a youth player for F.C. Scunthorpe United.

Property	Value
Name	?
Year of Birth	?
Place of Birth	?
Soccer Club	?

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Year of Birth	15/12/1977
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Soccer Club	?

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Property	Value
Name	Jack "Jacky" Miller
Year of Birth	15/12/1977
Place of Birth	?
Soccer Club	F.C. Scunthorpe United.

## **Knowledge Graphs to the Rescue!**



## Structured Prediction with Conditional Random Field (CRFs)

Probabilistic model of the probabilities of target variables given the text x:

$$p(\boldsymbol{y}|\boldsymbol{x};\theta)$$

Maximum-a-posteriori inference to determine most likely slot filling:

$$\vec{y}' = \operatorname*{argmax}_{\vec{y}} p(\vec{y}|\vec{x};\theta).$$

Property	Value
Name	Jack "Jacky" Miller
Year of Birth	15/12/1977
Place of Birth	?
Soccer Club	F.C. Scunthorpe United.

## **CRFs** with factor graphs

#### **Formal Definition**:

- A factor graph G consists of
  - random variables **x** and **y** (grey boxes)  $\bigcirc$
  - factors  $\Psi$  (black boxes).  $\bigcirc$

$$p(\boldsymbol{y}|\boldsymbol{x};\theta) = \frac{1}{Z(\boldsymbol{x})} \prod_{\boldsymbol{\Psi}_i \in \boldsymbol{\mathcal{G}}} \boldsymbol{\Psi}_i$$

Each factor computes a scalar score based on a feature vector  $f_i(\mathbf{x}_i, \mathbf{y}_i)$  and a set of parameters  $\theta_{i:}$ 

$$\Psi_i = e^{f_i(oldsymbol{x}_i,oldsymbol{y}_i)\cdot heta_i}$$



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### Incorporating Semantic Dependencies From Knowledge Graphs

Conditional Random Field:

$$p(\boldsymbol{y}|\boldsymbol{x};\theta) = \frac{1}{Z(\boldsymbol{x})} \prod_{\boldsymbol{\Psi}_i \in \boldsymbol{\mathcal{G}}} e^{f_i(\boldsymbol{x}_i,\boldsymbol{y}_i) \cdot \theta_i}$$

Query as feature function:

$$f_{s_i,s_j}(\hat{e}, e', p) = \begin{cases} 1 & \text{iff } p \in eval(Q(0)) \\ 0 & \text{else} \end{cases}$$



## Path Queries

1. Undirected-1-hop-relation:

 $Q_1(e_1, e_2) = \{e_1 ? r e_2\}$ 

2. Undirected-2-hop-relation:

$$Q_2(e_1, e_2) = \exists o \{ e_1 ? r_1 o \land o ? r_2 \}$$

3. Tail Plausibility:

$$Q_3(r, e_1) = \exists h \{h \ r \ e_1\}$$

4. V-relation:

 $Q_4(e_1, e_2) = \exists o \{ e_1 ? r_1 o \land e_2 ? r_2 o \}$ 



#### $e_2$

## Dotooto

	ald	ISE	LS	Dataset	Cardinality	Туре	Values
				SoccerPlayer			
<ul> <li>dbr:SoccerPlay</li> </ul>	/er (#2338)			resource birthPlace birthYear	single multi single	entity entity literal	4,905 2,314 n/a
<ul> <li>dbr:Film (#100)</li> <li>dbr:Single (#10)</li> <li>dbr:Architectur</li> <li>dbr:Dom (#401)</li> </ul>	0) )00) alStructure	(#527)		deathYear position team	single single multi	literal entity entity	n/a 14 4,359
• UDI.Dalli (#491	)			Film			
ARCHITECTURALSTR	UCTURE			resource	single	entity	5,405
ARCHITECTURALSTRUCTURresourcesingarchitectmuarchitecturalStylemulocationmuopeningYearsing		entity entity entity entity literal	530 356 70 408 n/a	producer director writer starring musicComposer distributor	multi multi multi multi multi	entity entity entity entity entity entity	3,347 5,452 5,452 9,452 731 1,936
yearOfConstruction	multi	Interal	n/a	SINGLE			-,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,
DAM resource sing river mul country mul location mul status sing openingYear mul		single entity 502 multi entity 370 multi entity 74 multi entity 601 single literal n/a multi literal n/a		resource writer musicalBand musicalArtist album producer	single multi multi multi multi multi	entity entity entity entity entity entity	17,881 7,001 4,791 4,791 10,090 4,185 548

## **Experiments on 5 datasets**

- Experiments were run 3 times with a random 80/20 (train/test) split
- We report averaged harmonic macro F1
- Baseline: pick entity as property value based on the frequency in the text
- Intra-textual Model: CRF that relies on textual features only
- Intra-textual + SD Model: CRF with KG dependencies on top of textual features

	I	Baseline	;	Intra-t	extual N	Model	Intra-textual + SD Model			
Dataset	prec.	rec.	$\mathbf{F}_1$	prec.	rec.	$\mathbf{F}_1$	prec.	rec.	$\mathbf{F}_1$	
SOCCERPLAYER	0.35	0.31	0.33	0.82	0.77	0.79	0.91	0.88	0.89	
Film	0.09	0.09	0.09	0.63	0.65	0.64	0.63	0.66	0.64	
SINGLE	0.11	0.12	0.11	0.62	0.64	0.61	0.70	0.79	0.74	
ARCH_STRUCT*	0.25	0.28	0.26	0.76	0.68	0.71	0.77	0.69	0.73	
DAM	0.39	0.42	0.40	0.80	0.66	0.72	0.80	0.68	0.73	
Average	0.24	0.24	0.24	0.72	0.67	0.70	0.76	0.74	0.75	

## **Ablation Experiments**

Model	precision	recall	$\mathbf{F}_1$
Lin+BK	0.76	0.74	0.75
Lin+BK - Q1	0.75	0.73	0.74
Lin+BK - Q <sub>2</sub>	0.74	0.70	0.72
Lin+BK - Q <sub>3</sub>	0.76	0.73	0.74
Lin+BK - Q <sub>4</sub>	0.77	0.73	0.75

## Interim Conclusions

- Background knowledge can be successfully integrated into a CRF model via indicator functions.
- 2. The integration shows a positive impact in the slot filling task. Up to 10% F1 for individual datasets. (SoccerPlayer)
- Ablation study shows that a wide variety of queries is important to retrieve information from the knowledge graph, two-hop dependencies being the most important.



# Scientific Knowledge Graphs

- **Definition:** A scientific knowledge graph is a knowledge graph that describes the body of research in some discipline!
- What are Scientific Knowledge Graphs good for?
  - Knowledge Exploration
  - Knowledge Aggregation (e.g. Scientific) Reviews, Meta-Analysis, ...)
  - Inconsistency Detection

#### 1st Workshop on Scientific Knowledge Graphs

February 25, 2020 | BY angelosalatino

Event Notification Type: Call for Papers Abbreviated Title: SKG2020

Tuesday, 25 August 2020 **Country:** France Contact Email: skg2020@easychair.org City: Lyon **Contact:** Angelo Salatino Andrea Mannocci Francesco Osborne Website: https://skg.kmi.open.ac.uk/SKG2020/ Submission Deadline: Saturday, 4 April 2020

web: https://skg.kmi.open.ac.uk, twitter: @skgworkshop

Held in conjunction with TPDL2020, 25th-28th August 2020, Lyon, France

## Knowledge aggregation in medicine

- Systematic reviews crucial for advance of knowledge in medicine, carried out since mid 70s
- Systematic reviews, meta-analysis, HTA require knowledge aggregation, currently done by hand (!)
- Outdated when they are published, although they are supposed to be updated, for most systematic reviews this is not the case
- 12 clinical trials per average in one systematic review => most clinical trials not "reviewed"

OPEN බ ACCESS Freely available online

PLOS MEDICINE

Policy Forum

#### Seventy-Five Trials and Eleven Systematic Reviews a Day: How Will We Ever Keep Up?

Hilda Bastian<sup>1</sup>\*, Paul Glasziou<sup>2</sup>, Iain Chalmers<sup>3</sup>

1 German Institute for Quality and Efficiency in Health Care (IQWiG), Cologne, Germany, 2 Centre for Research in Evidence-Based Practice, Faculty of Health Sciences, Bond University, Gold Coast, Australia, 3 James Lind Library, James Lind Initiative, Oxford, United Kingdom



Source: https://ClinicalTrials.gov

## **Registered Clinical Trials**







### **Extracting Outcomes from Pre-Clinical Literature**





### Spinal Cord Injury Ontology (SCIO) Organism Model



### Spinal Cord Injury Ontology (SCIO) Injury



#### Spinal Cord Injury Ontology (SCIO) Treatment



### Spinal Cord Injury Ontology (SCIO) Experimental Group



### Spinal Cord Injury Ontology (SCIO) Result



### Spinal Cord Injury Ontology (SCIO) Trend









# Spinal Cord Injury Ontology

- Model-Complete Text Comprehension (MCTC)
  - Interpret text with respect to a given (ontological) model
  - Extract only those things that are relevant for a given ontology
  - Ignore everything else
- Important Subproblem: predict cardinality (inference!)  $\bullet$

## **Problem Formulation**

### Model-complete text comprehension as structured (probabilistic) inference

- Assume we have an ontology with two classes:
  - Class A with properties hasProperty1, hasProperty2 and has Property3
  - Class **B** with properties hasProperty4, hasProperty5
- An instance of the model/ontology could be captured by the following vector:

 $(2,{(a_1,p_1,p_2,p_3),(a_2,p_1',p_2',p_3')},3,{(b_1,p_4,p_5),(b_2,p_4',p_5'),(b_3,p_4'',p_5'')})$ 

• Let Y be the set of all such vectors given a certain (ontological) vocabulary O. We get the most likely instance of our model by maximum-a-posteriori inference:

$$\vec{\mathbf{y}}' = \operatorname*{argma}_{\vec{y} \in \mathbf{Y}}$$

 $\operatorname{ax} p(\vec{y}|\vec{x}).$ 

## IE Architecture



unidirectional information flow

## Example target structure



## Annotated corpus

Corpus	#doc.	#ind	#itp	#etp	#ltp	#tri	#ett	#ltt
OrganismModel	200	216	0	3	2	1.006	571	219
INJURYDEVICE	165	169	0	0	8	270	0	101
DeliveryMethod	161	268	0	1	1	736	296	29
INJURYLOCATION	198	221	0	0	2	355	134	0
ANAESTHETIC	160	269	1	0	1	986	311	264
INJURY	199	220	3	0	0	2.308	1.150	363
TREATMENT	133	454	1	3	1	3.309	1.622	278
ExperimentalGroup	95	219	3	0	1	7.636	3.821	1.845
Trend	91	2.019	0	1	2	4.272	1.841	569
InvestigationMethod	91	843	0	0	0	843	0	0
Result	91	1.770	3	1	0	23.675	14.760	2.425
Overall (distinct)	200	6668	10	9	17	53.829	26.271	4.487

## Organism Model

## Adult male Wistar rats weighing 270-300 g were used in our experiments.

			т	U		~ I			
$ORGANISMMODEL^C$		joint			entity			relation	
Macro	$F_1$	Р	R	$F_1$	Р	R	$F_1$	Р	R
$hasWeight^L$	0.873	0.879	0.866	0.955	0.955	0.955	0.899	0.906	0.893
$hasAge^{L}$	0.681	0.712	0.654	0.957	0.957	0.957	0.662	0.684	0.640
$hasSpecies^E$	0.859	0.865	0.853	0.896	0.900	0.892	0.905	0.915	0.895
$has Age Category^E$	0.884	0.889	0.880	0.997	1.000	0.993	0.882	0.886	0.877
$has Gender^{E}$	0.962	0.972	0.952	0.994	0.994	0.994	0.962	0.972	0.952
cardinality	0.990	1.000	0.980	0.995	1.000	0.995	0.990	1.000	0.980
overall	0.913	0.944	0.884	0.971	0.995	0.948	0.924	0.935	0.914

# Type of Injury, Location and Device

#### SCI Balloon compression was used to create an SCI. A 2-french Fogarty catheter was inserted below T8, and the balloon was inflated with 15 LVolume saline for 5 min at T8.

$Injury^C$	joint		joint entity relation				$InjuryDevice^{C}$			joint			entity			relation				
Macro	$F_1$	Р	R	$F_1$	Р	R	$F_1$	Р	R		Macro	$F_1$	Р	R	$F_1$	Р	R	$F_1$	Р	R
$type^E$	0.596	0.610	0.583	0.992	0.995	0.990	0.595	0.610	0.580		$type^{E}$ has $Weiaht^{L}$	$\begin{array}{c} 0.686 \\ 0.641 \end{array}$	$\begin{array}{c} 0.689 \\ 0.641 \end{array}$	$\begin{array}{c} 0.683 \\ 0.641 \end{array}$	$\begin{array}{c} 0.886 \\ 0.683 \end{array}$	$\begin{array}{c} 0.890 \\ 0.683 \end{array}$	$\begin{array}{c} 0.881 \\ 0.683 \end{array}$	$\begin{array}{c} 0.777 \\ 0.511 \end{array}$	$\begin{array}{c} 0.780 \\ 0.511 \end{array}$	$\begin{array}{c} 0.774 \\ 0.511 \end{array}$
$has Injury Anaesthesia^{I*}$	0.383	0.476	0.320	0.412	0.518	0.341	0.804	0.983	0.680		$hasForce^{L}$	0.704	0.704	0.704	0.778	0.778	0.778	0.852	0.852	0.852
$has Injury Device^{I}$	0.652	0.644	0.660	0.662	0.652	0.672	0.928	0.934	0.922		$has Duration^L$	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
$has Injury Location^{I}$	0.708	0.721	0.695	0.726	0.728	0.724	0.956	0.980	0.934		$hasDistance^{L} \\ hasVolume^{L}$	$\begin{array}{c} 0.625 \\ 0.000 \end{array}$	$\begin{array}{c} 0.625 \\ 0.000 \end{array}$	$\begin{array}{c} 0.625 \\ 0.000 \end{array}$	$\begin{array}{c} 0.735 \\ 0.500 \end{array}$	$\begin{array}{c} 0.735 \\ 0.500 \end{array}$	$\begin{array}{c} 0.735 \\ 0.500 \end{array}$	$\begin{array}{c} 0.658 \\ 0.500 \end{array}$	$\begin{array}{c} 0.658 \\ 0.500 \end{array}$	$\begin{array}{c} 0.658 \\ 0.500 \end{array}$
cardinality	0.977	1.000	0.955	0.997	1.000	0.995	0.977	1.000	0.955		cardinality	0.966	0.976	0.957	0.966	0.976	0.957	0.966	0.976	0.957
overall	0.532	0.582	0.490	0.661	0.809	0.559	0.804	0.914	0.717		overall	0.704	0.702	0.705	0.866	0.890	0.843	0.777	0.765	0.789

InjuryLocation <sup><math>C</math></sup>		joint				relation			
Macro	$F_1$	Р	R	$F_1$	Р	R	$F_1$	Р	R
$type^E$	0.689	0.710	0.669	0.912	0.915	0.908	0.800	0.820	0.781
$has Upper Vertebrae^E$	0.471	0.471	0.471	0.838	0.838	0.838	0.632	0.632	0.632
$hasLowerVertebrae^{E}$	0.206	0.206	0.206	0.794	0.794	0.794	0.412	0.412	0.412
cardinality	0.979	1.000	0.959	0.997	1.000	0.993	0.979	1.000	0.959
overall	0.620	0.640	0.601	0.908	0.915	0.901	0.741	0.758	0.725

# Treatment, Delivery Method

A total of **3x105 OEG** and/or **MSC** was injected through a **glass pipette** at a concentration of 1x105 cells/L, into the **proximal, central and distal** parts of the lesioned spinal cord (each part received 1 L cell suspension), at a depth of 1 mm below the dorsal surface and a rate of 1 L/min using a **Nano-Injector** (Stoelt294 ing Co.); OEG/MSC-transplanted animals received **six injections** (3x105 OEG and 3 x105 MSC) instead of the three injections received by the other animals.

## The control group received three injections of saline (1 L), also into the proximal, central and distal parts of the lesioned spinal cord.

$\mathrm{Treatment}^C$	joint		entity		relation			$\text{DeliveryMethod}^C$	joint			entity			relation				
Macro	$F_1$	Р	R	$F_1$	Р	R	$F_1$	Р	R	Macro	$F_1$	Р	R	$F_1$	Р	R	$F_1$	р	
$has Delivery Method^{I}$	0.282	0.321	0.251	0.333	0.384	0.294	0.715	0.757	0.677		<u> </u>	•			-	10		-	
$has Direction^{E*}$	0.065	0.075	0.057	0.889	0.933	0.849	0.109	0.151	0.085	$type^{E}$	0.653	0.806	0.548	0.948	0.963	0.934	0.681	0.838	0.574
$has App. Instrument^E$	0.351	0.378	0.328	0.697	0.802	0.616	0.426	0.442	0.411	$has Duration^L$	0.000	0.000	0.000	0.053	0.053	0.053	0.000	0.000	0.000
$has Compound^E$	0.458	0.532	0.402	0.899	1.000	0.817	0.532	0.589	0.484	$has Locations^{E*}$	0.346	0.438	0.286	0.623	0.683	0.573	0.417	0.525	0.346
$has Dosage^L$	0.038	0.033	0.044	0.253	0.331	0.205	0.319	0.302	0.339										
cardinality	0.817	0.860	0.778	1.000	1.000	1.000	0.819	0.738	0.920	cardinality	0.818	0.975	0.705	0.948	0.963	0.934	0.834	1.000	0.715
overall	0.272	0.373	0.214	0.626	0.873	0.448	0.487	0.530	0.451	overall	0.485	0.622	0.398	0.782	0.848	0.725	0.536	0.681	0.441

## **Experimental Group**

#### The lesioned animals were divided into four groups. The first group received both OEG and MSC (n = 21).

Experimental $GROUP^{C}$		joint			entity				
Macro	$F_1$	Р	R	$F_1$	Р	R	$F_1$	Р	R
$has Organism Model^{I}$	0.605	0.614	0.597	0.627	0.634	0.620	0.748	0.748	0.748
$has Injury Model^{I}$	0.340	0.360	0.322	0.358	0.384	0.334	0.755	0.755	0.755
$has Treatment^{I*}$	0.180	0.200	0.164	0.239	0.273	0.213	0.559	0.562	0.557
$\rightarrow mainTreatment$	0.164	0.184	0.148	0.210	0.246	0.183	0.531	0.533	0.529
$\rightarrow subTreatment$	0.026	0.031	0.022	0.041	0.040	0.041	0.622	0.626	0.619
cardinality	0.838	0.762	0.931	0.903	1.000	0.823	0.897	0.863	0.935
overall	0.377	0.422	0.341	0.450	0.538	0.387	0.720	0.729	0.711



# Results, Investigation Method

The control animals achieved BBB scores of 7.08 +/- 0.24 at the end of the experiment (9 weeks after SCI, 8 weeks after transplantation) but never supported their body weight on their hind legs. Animals with OEG and MSC co-grafts, even though they received six injections, showed a statistically significant improvement 6 weeks after SCI, with **BBB** of 9.18 +/-0.44.

$\operatorname{Result}^C$	joint				_	entity		relation			
Macro	$F_1$	Р	R		$F_1$	Р	R	$F_1$	Р	R	
$has Investigation Method^E$	0.229	0.274	0.196		0.714	0.884	0.598	0.711	0.714	0.708	
$has Trend^{I}$	0.186	0.392	0.122		0.716	0.902	0.593	0.638	0.665	0.613	
$has Target Group^{I}$	0.342	0.471	0.268		0.560	0.623	0.509	0.837	0.827	0.847	
$has Reference Group^{I}$	0.351	0.501	0.270		0.574	0.625	0.531	0.822	0.830	0.813	
cardinality	0.628	0.779	0.526		1.000	1.000	1.000	0.860	0.861	0.860	
overall	0.333	0.475	0.257		0.576	0.645	0.520	0.830	0.830	0.830	

- SCIExplorer: <u>http://psink.techfak.uni-bielefeld.de/SCIExplorer/</u>
- Rationalizing Medical Evidence via Argumentation: <u>http://</u> scdemo.techfak.uni-bielefeld.de/ratio-argviz/
- grading/kwon/

## **Prototype Applications**

Automatic Grading of Therapies: <u>http://psink.techfak.uni-bielefeld.de/</u>

# Summary

- Background knowledge in knowledge graphs can enhance / improve NLP
- Hypothesis: Scientific Knowledge Graphs will play a key role in reaching FAIR scientific knowledge dissemination
- NLP methods crucial to bootstrap the creation of scientific knowledge graphs
- Challenge: requires deep discipline-specific ontologies and NLP systems to extract fine-grained knowledge following these ontologie

### Thanks for your attention!

- Dr. Olivia Sánchez-Graillet
- Hendrik ter Horst
- Frank Grimm
- Christian Grimm
- Dr. Roman Klinger
- Prof. Dr. Werner Müller
- Dr. Nicole Brazda







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