

# Introduction to Graph Neural Networks with an application to Knowledge Graphs

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24 March 2021

# Talk outline

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- ▶ Why Graph Neural Networks matter
- ▶ Neural Networks - key concepts
- ▶ Graph Neural Networks
  - ▶ What are they?
  - ▶ How do they work?
  - ▶ What can they do?
- ▶ Knowledge graphs

# Why Graph Neural Networks matter...

...they matter for 300+ reasons...

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- ▶ Reason 1: GNNs save lives!

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- ▶ Reason 1: GNNs save lives!
- ▶ Reason 2: GNNs solve the Traveling Salesperson Problem  
(sort of...)

# Why Graph Neural Networks matter...

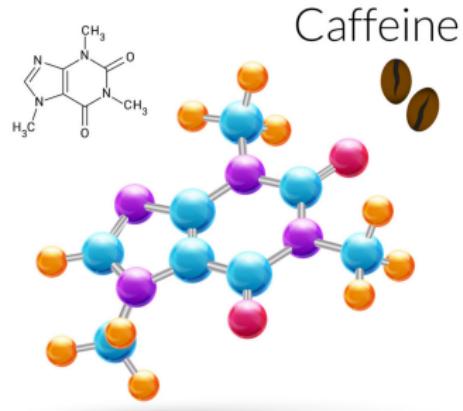
...they matter for 300+ reasons...we will list 3:

- ▶ Reason 1: GNNs save lives!
- ▶ Reason 2: GNNs solve the Traveling Salesperson Problem  
(sort of...)
- ▶ Reason 3: GNNs are the future of AI...

# Why Graph Neural Networks matter...

## Reason 1: GNNs save lives!

- ▶ Molecules are graphs...
- ▶ ....atoms as nodes, bonds as edges
- ▶ apply GNN to predict whether a molecule is a candidate for a drug



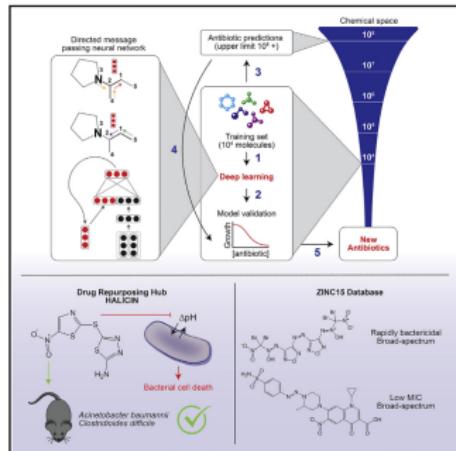
# Why Graph Neural Networks matter...

Cell

Article

## A Deep Learning Approach to Antibiotic Discovery

### Graphical Abstract



### Authors

Jonathan M. Stokes, Kevin Yang,  
Kyle Swanson, ..., Tommi S. Jaakkola,  
Regina Barzilay, James J. Collins

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### In Brief

A trained deep neural network predicts antibiotic activity in molecules that are structurally different from known antibiotics, among which Halicin exhibits efficacy against broad-spectrum bacterial infections in mice.

### Highlights

- A deep learning model is trained to predict antibiotics based on structure

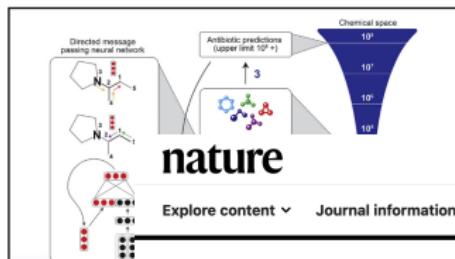
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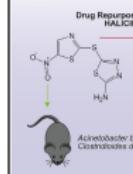
### Correspondence

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NEWS • 20 FEBRUARY 2020

## Powerful antibiotics discovered using AI

Machine learning spots molecules that work even against 'untreatable' strains of bacteria.

Jo Marchant

### Highlights

- A deep learning on structure



# Why Graph Neural Networks matter...

Reason 2: GNNs (almost) solve  
the Traveling Salesperson Prob-  
lem

# Why Graph Neural Networks matter...

Reason 2: GNNs (almost) solve the Traveling Salesperson Problem

Published as a conference paper at ICLR 2019

## ATTENTION, LEARN TO SOLVE ROUTING PROBLEMS!

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### ABSTRACT

The recently presented idea to learn heuristics for combinatorial optimization problems is promising as it can save costly development. However, to push this idea towards practical implementation, we need better models and better ways of training. We contribute in both directions: we propose a model based on attention layers with benefits over the Pointer Network and we show how to train this model using REINFORCE with a simple baseline based on a deterministic greedy rollout, which we find is more efficient than using a value function. We significantly improve over recent learned heuristics for the Travelling Salesman Problem (TSP), being able to obtain results for problems up to 100 nodes. With these hyperparameters, we learn strong heuristics for three variants of the Vehicle Routing Problem (VRP), the Orienteering Problem (OP) and (a stochastic variant of) the Prize Collecting TSP (PCTSP), outperforming a wide range of baselines and getting results close to highly optimized and specialized algorithms.

- ▶ TSP problem is NP-hard, but not that hard for GNNs...
- ▶ "...getting close to optimal results for problems up to 100 nodes..."

# Why Graph Neural Networks matter...

## Reason 3: GNNs are the path to General AI...

Relational inductive biases, deep learning, and graph networks

Peter W. Battaglia<sup>1\*</sup>, Jessica B. Hamrick<sup>1</sup>, Victor Bapst<sup>1</sup>,  
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Daan Wierstra<sup>1</sup>, Pushmeet Kohli<sup>1</sup>, Matt Botvinick<sup>1</sup>,  
Oriol Vinyals<sup>1</sup>, Yujia Li<sup>1</sup>, Razvan Pascanu<sup>1</sup>

<sup>1</sup>DeepMind; <sup>2</sup>Google Brain; <sup>3</sup>MIT; <sup>4</sup>University of Edinburgh

### Abstract

Artificial intelligence (AI) has undergone a renaissance recently, making major progress in key domains such as vision, language, control, and decision-making. This has been due, in part, to cheap data and cheap compute resources, which have fit the natural strengths of deep learning. However, many defining characteristics of human intelligence, which developed under much different pressures, remain out of reach for current approaches. In particular, generalizing beyond one's experiences—a hallmark of human intelligence from infancy—remains a formidable challenge for modern AI.

The following is part position paper, part review, and part unification. We argue that combinatorial generalization must be a top priority for AI to achieve human-like abilities, and that structured representations and computations are key to realizing this objective. Just as biology uses nature and nurture cooperatively, we reject the false choice between “hand-engineering”

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- ▶ *"We argue that combinatorial generalization must be a top priority for AI to achieve human-like abilities, and that structured representations and computations are key to realizing this objective."*

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## Intro to DeepMind's Graph-Nets

A short overview of the core components of Graph-Nets



Kristof Neys Jan 20 · 7 min read

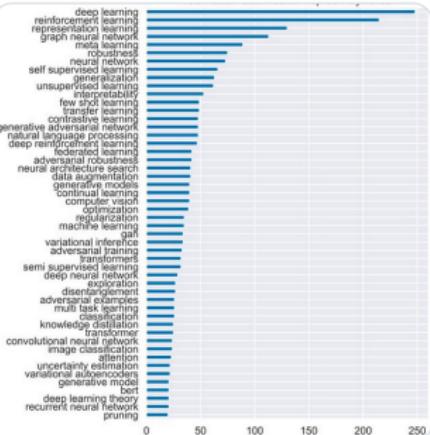


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es, and that  
is are key to*

# No surprise then: GNNs are HOT...

 Christopher Manning  
@chrmanning 

The amazing rise of reinforcement learning!  
(With graph neural networks and meta-learning  
in hot pursuit. ConvNets? Tired.) Based on  
**#ICLR2021** keywords HT @PetarV\_93



Keyword	Count
reinforcement learning	220
representation learning	180
graph neural network	140
meta-learning	120
robustness	100
neural network	90
self-supervised learning	80
generalization	70
unsupervised learning	60
interpretability	50
few shot learning	45
transfer learning	40
contrastive learning	35
generative models	30
natural language processing	28
deep reinforcement learning	25
adversarial training	22
adversarial robustness	20
neural architecture search	18
data augmentation	16
generative models	14
computer vision	12
regularization	10
machine learning	8
gan	6
variational inference	5
ablation studies	4
transformers	3
semi-supervised learning	2
deep neural network	1
exploration	1
discrepancy	1
adversarial examples	1
multi-task learning	1
classification	1
knowledge distillation	1
convolutional neural network	1
image classification	1
attention	1
uncertainty estimation	1
variational autoencoder	1
generative model	1
deep learning theory	1
recurrent neural network	1
pruning	1

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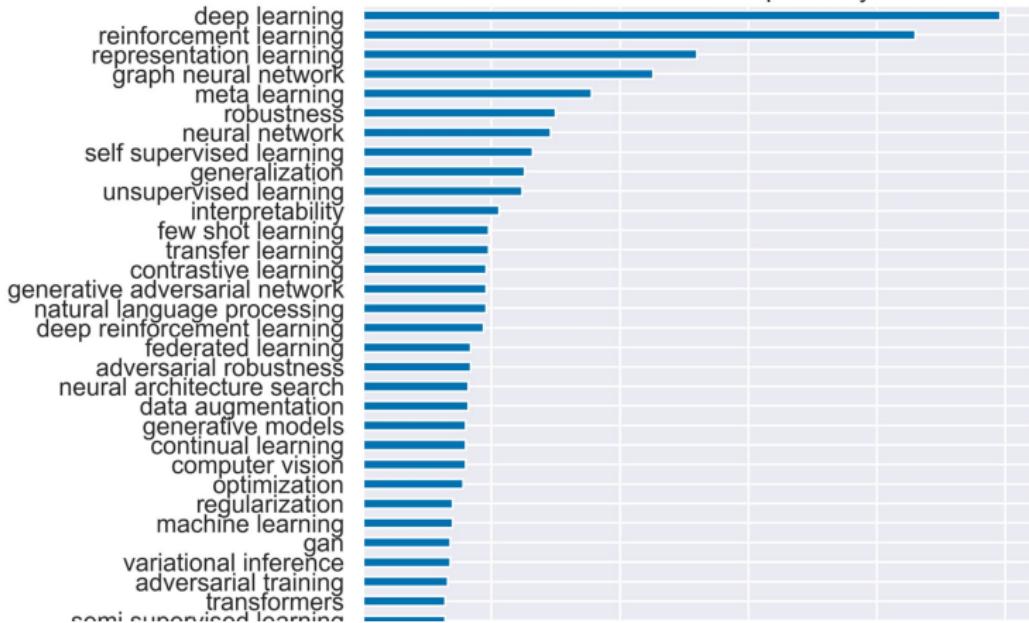


Christopher Manning  
@chrmanning



The amazing rise of reinforcement learning!  
(With graph neural networks and meta-learning  
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ICLR 2021 Submission Top 50 Keywords

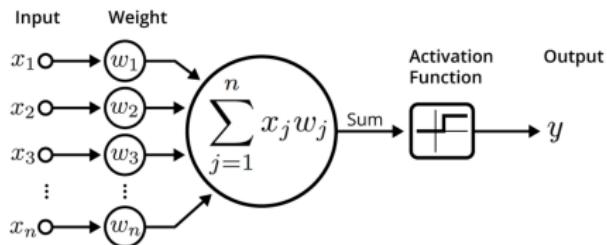


# Review of Neural Networks

# Neural Networks

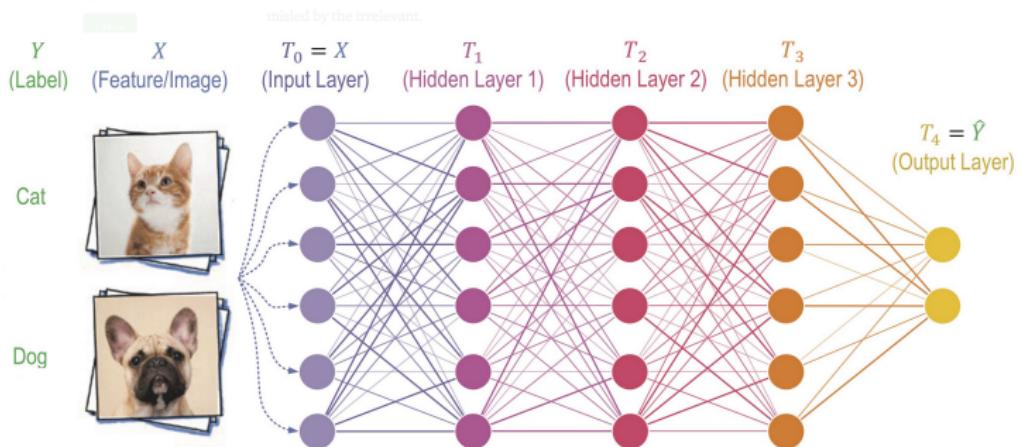
- ▶ Basic intuition is one of a succession of increasingly refined **data filters**
- ▶ Two key components: **artificial neuron** and **layer**
- ▶ The **artificial neuron** is an information processing unit taking in a set of inputs which are multiplied by numerical weights
- ▶ A series of these neurons can be stacked in a single **layer**
- ▶ A **Multilayer Perceptron** (MLP) combines several layers to perform an output prediction

# An Artificial Neuron



- ▶ Receive a list of numbers as input,  $x_i$ ;
- ▶ Multiply each number in the list by its weight,  $w_i$ ;
- ▶ Add up all of the results to get a single number
- ▶ Apply a non-linear *activation function*
- ▶ The weights,  $w_i$ , are the learnable parameters

# Neural Networks - Cat or Dog?



- ▶ Training data will only give a label for the final output layer (i.e. Cat, Dog). The intermediate layers are called *hidden layers*
- ▶ The neural network **learns** through measuring the output against a *loss function* and updating the weight parameters using the *backpropagation algorithm*

# Brain or Machine?



85 billion neurons...

# Brain or Machine?



85 billion neurons...



...175 billion parameters

# Graph Neural Networks

# Graph Neural Networks

- ▶ What are they?

# Graph Neural Networks

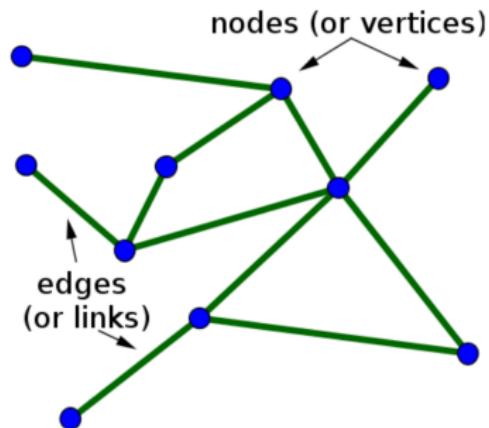
- ▶ What are they?
- ▶ How do they work?

# Graph Neural Networks

- ▶ What are they?
- ▶ How do they work?
- ▶ What can they do?

# Graphs

- ▶  $G = (V, E)$
- ▶  $V$  being the set of nodes,  
and  $E$  the set of edges



# Graph Neural Networks - what are they?

- ▶ The core idea is to generate **representations of nodes** that actually depend on the structure of the graph, as well as any feature information we might have

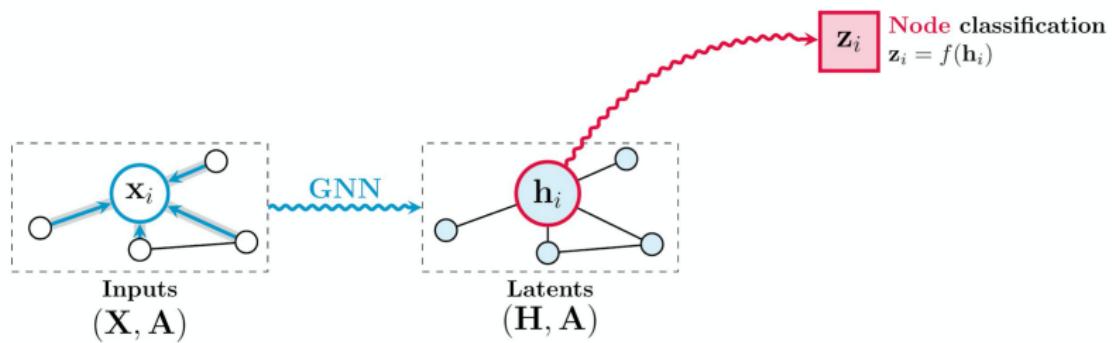
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- ▶ The key challenge is that the usual deep learning methods as illustrated on the previous slides only work on Euclidean data, i.e grid-like or sequential data structures

# Graph Neural Networks - what are they?

- ▶ The core idea is to generate **representations of nodes** that actually depend on the structure of the graph, as well as any feature information we might have
- ▶ The key challenge is that the usual deep learning methods as illustrated on the previous slides only work on Euclidean data, i.e grid-like or sequential data structures
- ▶ The essence of GNNs is the **message passing framework** upon which most GNNs are based

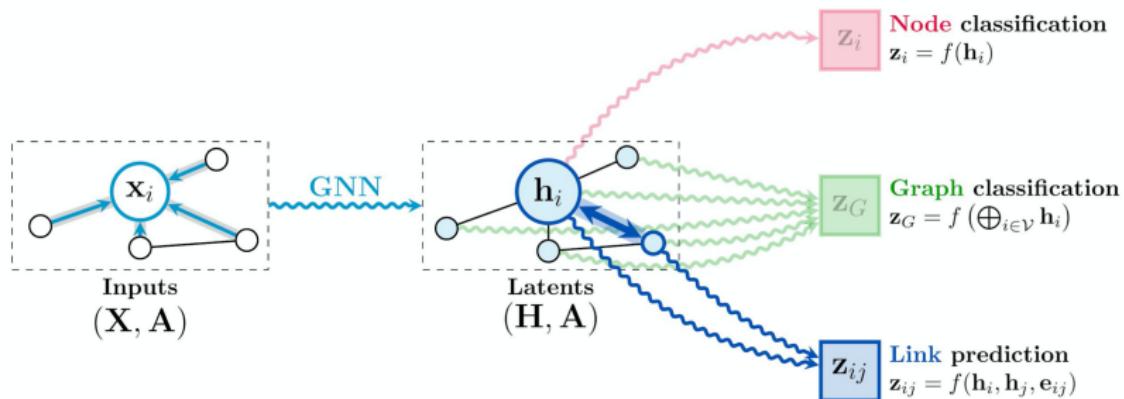
# Graph Neural Networks



1

<sup>1</sup>image by Dr. Petar Veličković

# Graph Neural Networks



2

<sup>2</sup>image by Dr. Petar Veličković

# Graph Neural Networks - definition & workings

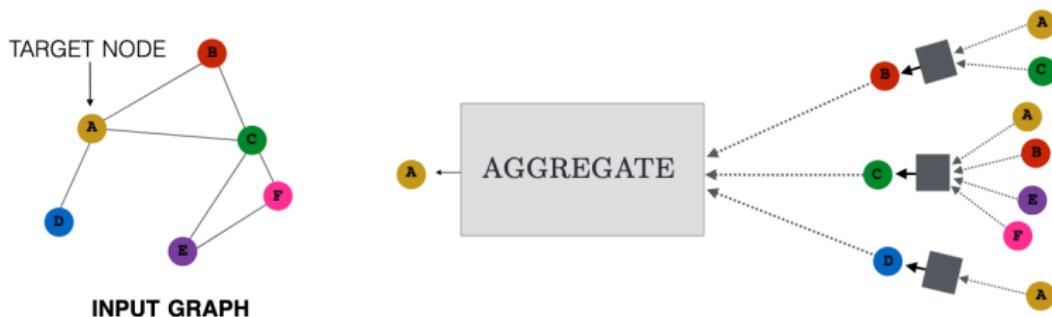
## Definition (Graph Neural Network)

Graph neural networks (GNNs) are a class of NN models suitable for processing graph structured data

- ▶ The architecture of a GNN is structured according to a graph  $G = (V, E)$
- ▶ A GNN takes as input an instance of a graph,  $G$ , where the nodes are associated with feature vectors,  $x_i$ ; and edges can also be associated with feature vectors;  $x_{ij}$
- ▶ **Hidden representations** of the nodes and edges in the neural network are denoted by  $h_i$  and  $h_{ij}$ , respectively.
- ▶ A *message passing* update is executed in sequence to obtain updated node and edge representations  $h'_i$  and  $h'_{ij}$ , respectively.

# GNN - How do they work?

- ▶ Core idea: during each **message passing iteration** in a GNN a hidden embedding  $h_a^{(k)}$ ,  $a \in V$ , is **updated** according to information **aggregated** from  $a$ 's graph neighborhood  $\mathcal{N}(a)$ .



# GNN - Message Passing framework

- ▶ The basic intuition is that at each iteration, ( $k$ ), every node aggregates information from its local neighborhood

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# GNN - Message Passing framework

- ▶ The basic intuition is that at each iteration, ( $k$ ), every node aggregates information from its local neighborhood
- ▶ The key functions are the UPDATE and AGGREGATE functions. It's the UPDATE function that provides trainable parameter matrices, equivalent to the MLP framework
- ▶ In essence, we are learning a mapping between a feature vector, which is an embedding of the neighbourhood of a node, and the label associated with that node.

# GNN - Message Passing framework

- ▶ Formally, this is represented as follows:

$$h_a^{(k+1)} = \text{UPDATE}^k \left( h_a^{(k)}, \text{AGGREGATE}^k \left( h_v^{(k)}, \forall v \in \mathcal{N}(a) \right) \right)$$

where UPDATE and AGGREGATE are differentiable functions.

# GNN - Message Passing framework

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where UPDATE and AGGREGATE are differentiable functions.

- ▶ Let  $m_{\mathcal{N}(a)}$  be the "*message*" that is aggregated from  $a$ 's neighborhood  $\mathcal{N}(a)$ , then:

$$m_{\mathcal{N}(a)} = \text{AGGREGATE}^k \left( h_v^{(k)}, \forall v \in \mathcal{N}(a) \right)$$

# GNN - Message Passing framework

- ▶ The UPDATE function combines  $m_{\mathcal{N}_{(a)}}$  with the previous embedding  $h_a^k$  of node  $a$  and computes  $h_a^{k+1}$
- ▶ UPDATE, in the basic GNN is defined as:

$$\sigma \left( W_a h_a + W_{neigh} m_{\mathcal{N}_{(a)}} \right)$$

- ▶  $W_a$  and  $W_{neigh}$  form the trainable weight matrices
- ▶ The prediction gets measured in a loss function and a backpropagation algorithm is applied to update the weight matrices

# Aggregate & Update define the GNN

Name	Variant	Aggregator	Updater
Spectral Methods	ChebNet	$\mathbf{N}_k = \mathbf{T}_k(\tilde{\mathbf{L}})\mathbf{X}$	$\mathbf{H} = \sum_{k=0}^K \mathbf{N}_k \Theta_k$
	1 <sup>st</sup> -order model	$\mathbf{N}_0 = \mathbf{X}$ $\mathbf{N}_1 = \mathbf{D}^{-\frac{1}{2}} \mathbf{A} \mathbf{D}^{-\frac{1}{2}} \mathbf{X}$	$\mathbf{H} = \mathbf{N}_0 \Theta_0 + \mathbf{N}_1 \Theta_1$
	Single parameter	$\mathbf{N} = (\mathbf{I}_N + \mathbf{D}^{-\frac{1}{2}} \mathbf{A} \mathbf{D}^{-\frac{1}{2}}) \mathbf{X}$	$\mathbf{H} = \mathbf{N} \Theta$
	GCN	$\mathbf{N} = \tilde{\mathbf{D}}^{-\frac{1}{2}} \tilde{\mathbf{A}} \tilde{\mathbf{D}}^{-\frac{1}{2}} \mathbf{X}$	$\mathbf{H} = \mathbf{N} \Theta$
Non-spectral Methods	Neural FPs	$\mathbf{h}_{\mathcal{N}_v}^t = \mathbf{h}_v^{t-1} + \sum_{k \in \mathcal{N}_v}^{\mathcal{N}_v} \mathbf{h}_k^{t-1}$	$\mathbf{h}_v^t = \sigma(\mathbf{h}_{\mathcal{N}_v}^t, \mathbf{W}_L^{\mathcal{N}_v})$
	DCNN	Node classification: $\mathbf{N} = \mathbf{P}^* \mathbf{X}$	$\mathbf{H} = f(\mathbf{W}^e \odot \mathbf{N})$
		Graph classification: $\mathbf{N} = \mathbb{1}_{\mathcal{N}}^T \mathbf{P}^* \mathbf{X} / N$	
	GraphSAGE	$\mathbf{h}_{\mathcal{N}_v}^t = \text{AGGREGATE}_t(\{\mathbf{h}_u^{t-1}, \forall u \in \mathcal{N}_v\})$	$\mathbf{h}_v^t = \sigma(\mathbf{W}^t \cdot [\mathbf{h}_v^{t-1}    \mathbf{h}_{\mathcal{N}_v}^t])$
Graph Attention Networks	GAT	$\alpha_{vb} = \frac{\exp(\text{LeakyReLU}(\mathbf{a}^T (\mathbf{W}\mathbf{h}_v    \mathbf{W}\mathbf{h}_b)))}{\sum_{j \in \mathcal{N}_v} \exp(\text{LeakyReLU}(\mathbf{a}^T (\mathbf{W}\mathbf{h}_v    \mathbf{W}\mathbf{h}_j)))}$ $\mathbf{h}_{\mathcal{N}_v}^t = \sigma(\sum_{k \in \mathcal{N}_v} \alpha_{vk} \mathbf{W}\mathbf{h}_k)$	
		Multi-head concatenation: $\mathbf{h}_{\mathcal{N}_v}^t = \left\  \begin{matrix} M \\ \alpha_{v1} \mathbf{W}^1 \mathbf{h}_v \\ \vdots \\ \alpha_{vM} \mathbf{W}^M \mathbf{h}_v \end{matrix} \right\ _{\text{concat}}$	
		Multi-head average: $\mathbf{h}_{\mathcal{N}_v}^t = \sigma\left(\frac{1}{M} \sum_{m=1}^M \sum_{k \in \mathcal{N}_v} \alpha_{vk}^m \mathbf{W}^m \mathbf{h}_k\right)$	
			$\mathbf{h}_v^t = \mathbf{h}_{\mathcal{N}_v}^t$
Gated Graph Neural Networks	GGNN	$\mathbf{h}_{\mathcal{N}_v}^t = \sum_{k \in \mathcal{N}_v} \mathbf{h}_k^{t-1} + \mathbf{b}$	$\mathbf{z}_v^t = \sigma(\mathbf{W}^z \mathbf{h}_{\mathcal{N}_v}^t + \mathbf{U}^z \mathbf{h}_v^{t-1})$ $\mathbf{r}_v^t = \sigma(\mathbf{W}^r \mathbf{h}_{\mathcal{N}_v}^t + \mathbf{U}^r \mathbf{h}_v^{t-1})$ $\mathbf{h}_v^t = \tanh(\mathbf{W}^h \mathbf{h}_{\mathcal{N}_v}^t + \mathbf{U}^h \mathbf{h}_v^{t-1})$ $\mathbf{h}_v^t = (1 - \mathbf{z}_v^t) \odot \mathbf{h}_v^{t-1} + \mathbf{z}_v^t \odot \mathbf{h}_v^t$
		$\mathbf{h}_{\mathcal{N}_v}^t = \sum_{k \in \mathcal{N}_v} \mathbf{h}_k^{t-1}$	$\mathbf{i}_v^t = \sigma(\mathbf{W}^i \mathbf{x}_v^t + \mathbf{U}^i \mathbf{h}_{\mathcal{N}_v}^t + \mathbf{b}^i)$ $\mathbf{f}_v^t = \sigma(\mathbf{W}^f \mathbf{x}_v^t + \mathbf{U}^f \mathbf{h}_{\mathcal{N}_v}^t + \mathbf{b}^f)$ $\mathbf{o}_v^t = \sigma(\mathbf{W}^o \mathbf{x}_v^t + \mathbf{U}^o \mathbf{h}_{\mathcal{N}_v}^t + \mathbf{b}^o)$ $\mathbf{u}_v^t = \tanh(\mathbf{W}^u \mathbf{x}_v^t + \mathbf{U}^u \mathbf{h}_{\mathcal{N}_v}^t + \mathbf{b}^u)$ $\mathbf{c}_v^t = \mathbf{i}_v^t \odot \mathbf{u}_v^t + \sum_{k \in \mathcal{N}_v} \mathbf{f}_v^t \odot \mathbf{c}_k^{t-1}$ $\mathbf{h}_v^t = \mathbf{o}_v^t \odot \tanh(\mathbf{c}_v^t)$
		$\mathbf{h}_{\mathcal{N}_v}^t = \sum_{k=1}^K \mathbf{U}_k^t \mathbf{h}_v^{t-1}$ $\mathbf{h}_{\mathcal{N}_v}^{ij} = \sum_{k=1}^K \mathbf{U}_{kij}^t \mathbf{h}_v^{t-1}$ $\mathbf{h}_{\mathcal{N}_v}^{jk} = \sum_{l=1}^L \mathbf{U}_{jl}^t \mathbf{h}_{\mathcal{N}_v}^{il}$ $\mathbf{h}_{\mathcal{N}_v}^t = \sum_{l=1}^L \mathbf{U}_{tl}^t \mathbf{h}_{\mathcal{N}_v}^{il}$	$\mathbf{i}_v^t = \sigma(\mathbf{W}^i \mathbf{x}_v^t + \mathbf{h}_{\mathcal{N}_v}^{ti} + \mathbf{b}^i)$ $\mathbf{f}_{vk}^t = \sigma(\mathbf{W}^f \mathbf{x}_v^t + \mathbf{h}_{\mathcal{N}_v}^{tf} + \mathbf{b}^f)$ $\mathbf{o}_{jk}^t = \sigma(\mathbf{W}^o \mathbf{x}_v^t + \mathbf{h}_{\mathcal{N}_v}^{to} + \mathbf{b}^o)$ $\mathbf{u}_{jk}^t = \tanh(\mathbf{W}^u \mathbf{x}_v^t + \mathbf{h}_{\mathcal{N}_v}^{tu} + \mathbf{b}^u)$ $\mathbf{c}_{jk}^t = \mathbf{i}_{jk}^t \odot \mathbf{u}_{jk}^t + \sum_{l=1}^L \mathbf{f}_{lk}^t \odot \mathbf{c}_{kl}^{t-1}$ $\mathbf{h}_v^t = \mathbf{o}_{jk}^t \odot \tanh(\mathbf{c}_{jk}^t)$
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The message passing framework is analogous to a standard MLP as it relies on linear operations followed by an activation function

- ▶ we first sum the messages incoming from the neighbours
- ▶ we combine the neighborhood information with the node's previous embedding using a linear combination
- ▶ apply an elementwise nonlinearity, i.e. an activation function

# GNNs - What can they do?

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- ▶ link (i.e. edge) prediction
- ▶ graph classification

## Example: Graph Attention Networks

- ▶ Cora dataset; the MNIST of graph land
  - ▶ 2708 academic papers, 7 classes ("Theory", "Reinforcement learning", "Probabilistic methods", ...) 5429 edges = citations, 1433 feature vector per node extracted from the text
  - ▶ only give 140 labeled nodes to train on (20 per class)
  - ▶ use GNN to predict the classes on 1000 nodes
- ▶ Semi-supervised learning to perform node classification

## GNNs - performance on Cora dataset

Method	Cora
MLP	55.1%
ManiReg (Belkin et al., 2006)	59.5%
SemiEmb (Weston et al., 2012)	59.0%
LP (Zhu et al., 2003)	68.0%
DeepWalk (Perozzi et al., 2014)	67.2%
ICA (Lu & Getoor, 2003)	75.1%
Planetoid (Yang et al., 2016)	75.7%
Chebyshev (Defferrard et al., 2016)	81.2%
GCN (Kipf & Welling, 2017)	81.5%
MoNet (Monti et al., 2016)	81.7 ± 0.5%
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- ▶ State-of-the-Art GNNs offer 28% improvement over MLPs...

# Graph Attention Network

## Neo4j & DGL — a seamless integration

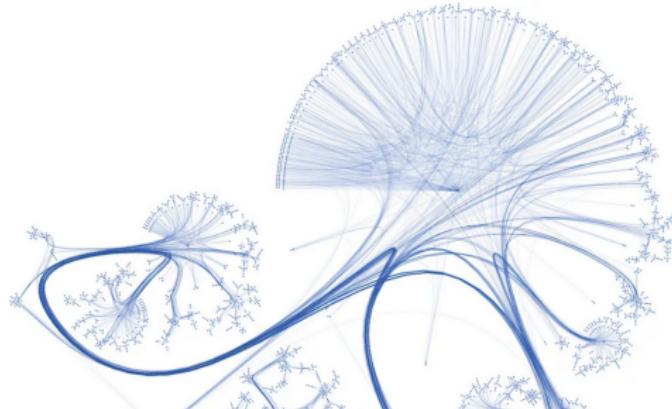
In this article we will illustrate how to integrate a Graph Attention Network model using the Deep Graph Library into the Neo4j workflow and deploying the Neo4j Python driver.



Kristof Neys Mar 5 · 11 min read



*This blog post was co-authored with [Clair Sullivan](#) and [Mark Needham](#)*



# Graph Attention Network

The screenshot shows a Jupyter Notebook interface with the following details:

- Title Bar:** Neo4j\_DGL\_Cora.ipynb
- Menu Bar:** File, Edit, View, Insert, Runtime, Tools, Help. A message "Changes will not be saved" is displayed.
- Toolbar:** Table of contents, X, + Code, + Text, Copy to Drive.
- Table of Contents:** Shows a list of sections and code cells, with the first cell expanded.
- Code Cell Content:**

```
This note book accompanies the article:  
Neo4j & DGL – a seamless integration,  
and implements a Graph Attention  
Network, (Veličković et al., ICLR 2018):  
https://arxiv.org/abs/1710.10903, using  
the Deep Graph Library, DGL, with  
TensorFlow 2.x as backend and Neo4j to  
write and store the graph
```
- Text Cell Content:**

```
Writing results back to Neo4j using Python  
drivers
```
- Section Cell Content:**

```
# To ensure that DGL can access GPU hardware; make sure to install CUDA10,
```

# Knowledge Graphs

# Knowledge Graphs

Christopher Strachey in letter to Alan Turing

*"I am convinced that the crux of the problem of learning is recognizing relationships and being able to use them"*

# Knowledge graphs

## Definition (Knowledge graphs)

A knowledge graph is a structured representation of facts, consisting of entities, relationships and semantic descriptions

- ▶ Entities can be real-world objects and abstract concepts

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- ▶ Entities can be real-world objects and abstract concepts
- ▶ Relationships represent the relation between entities
- ▶ Semantic description of the entities and relationships contain types and properties with a well-defined meaning
- ▶ A knowledge graph is a graphical representation of a knowledge base
- ▶ A knowledge base is in the form of **Resource Description Framework**, i.e. (Elon\_Musk, makes, cars), or **Property Graph**

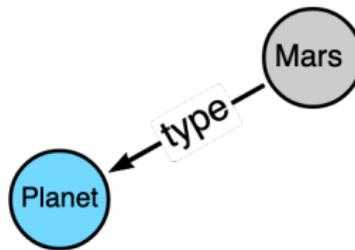
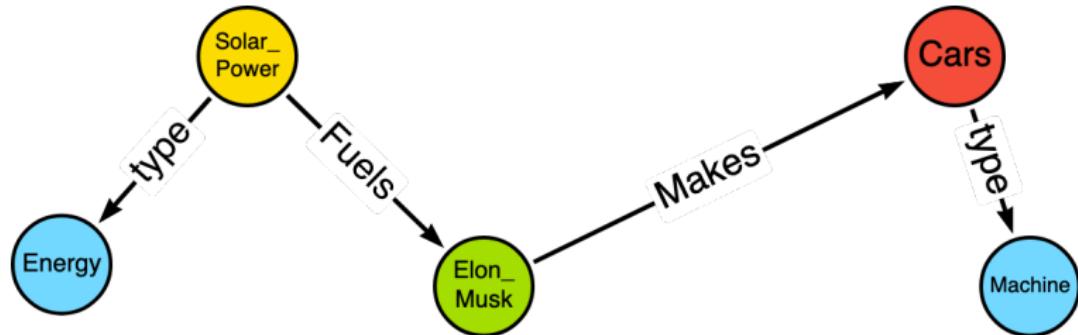
## KG + ML = a marriage made in heaven...

- ▶ Developing machine learning models is important since even the largest knowledge bases are incomplete and as such the gap in knowledge limit the downstream applications

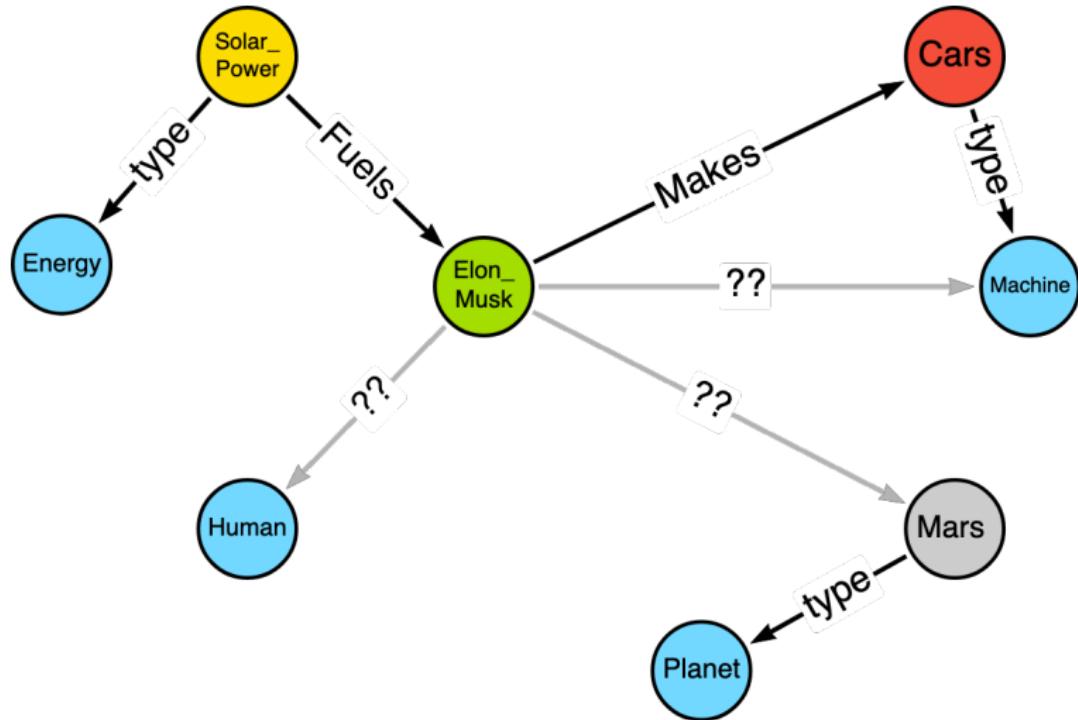
## KG + ML = a marriage made in heaven...

- ▶ Developing machine learning models is important since even the largest knowledge bases are incomplete and as such the gap in knowledge limit the downstream applications
- ▶ Predicting missing information in knowledge bases using machine learning is "**Statistical Relational Learning**" , a subfield of ML that deals with learning with relational structure

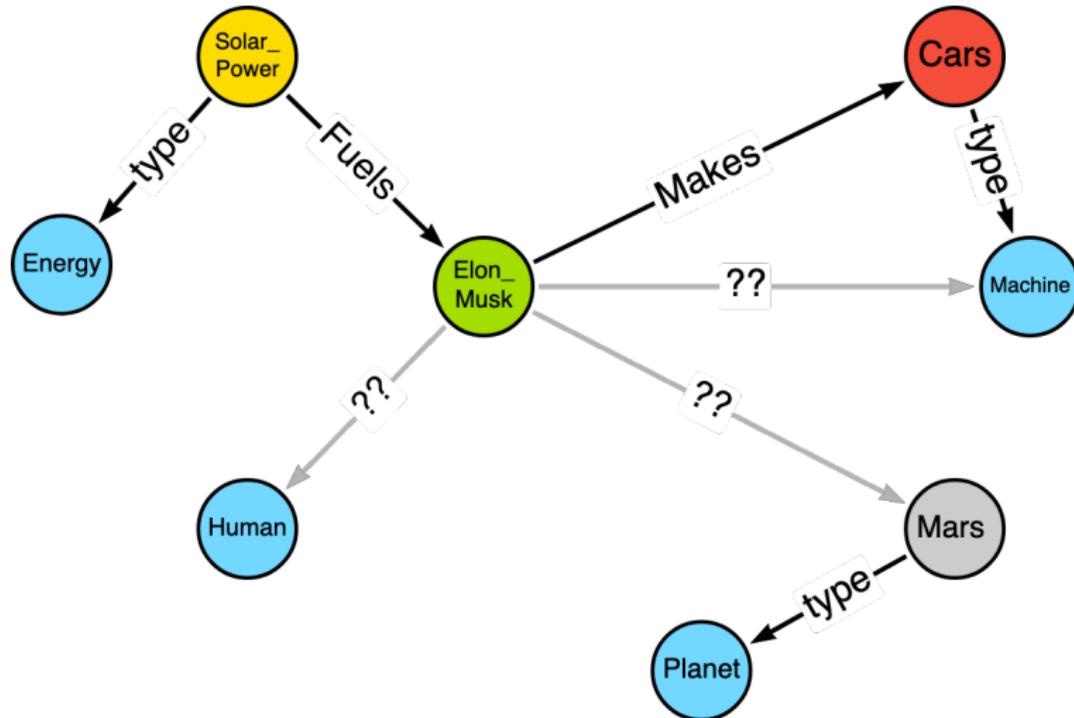
# Simplifying...



# Knowledge graph completion

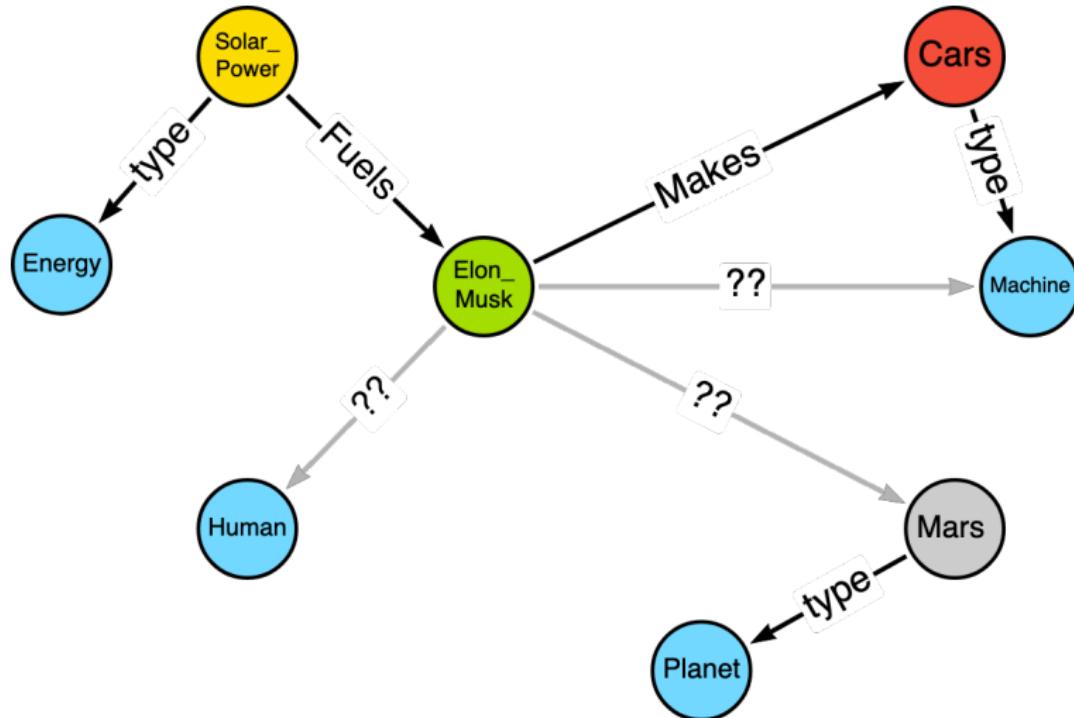


# Knowledge graph completion



► Elon Musk.... Human or Machine?

# Knowledge graph completion



- ▶ Elon Musk.... Human or Machine?
- ▶ ...born on Mars, Holiday...?

# Knowledge graphs - history

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# Knowledge graphs - history

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 $\infty\ldots$



**Alan Turing** ◀  
Mathematician

Alan Mathison Turing OBE FRS was an English mathematician, computer scientist, logician, cryptanalyst, philosopher, and theoretical biologist. [Wikipedia](#)

**Born:** 23 June 1912, Maida Vale, London  
**Died:** 7 June 1954, Wilmslow  
**Education:** Princeton University (1936–1938), [MORE](#)  
**Known for:** Cryptanalysis of the Enigma, Turing's proof, [MORE](#)

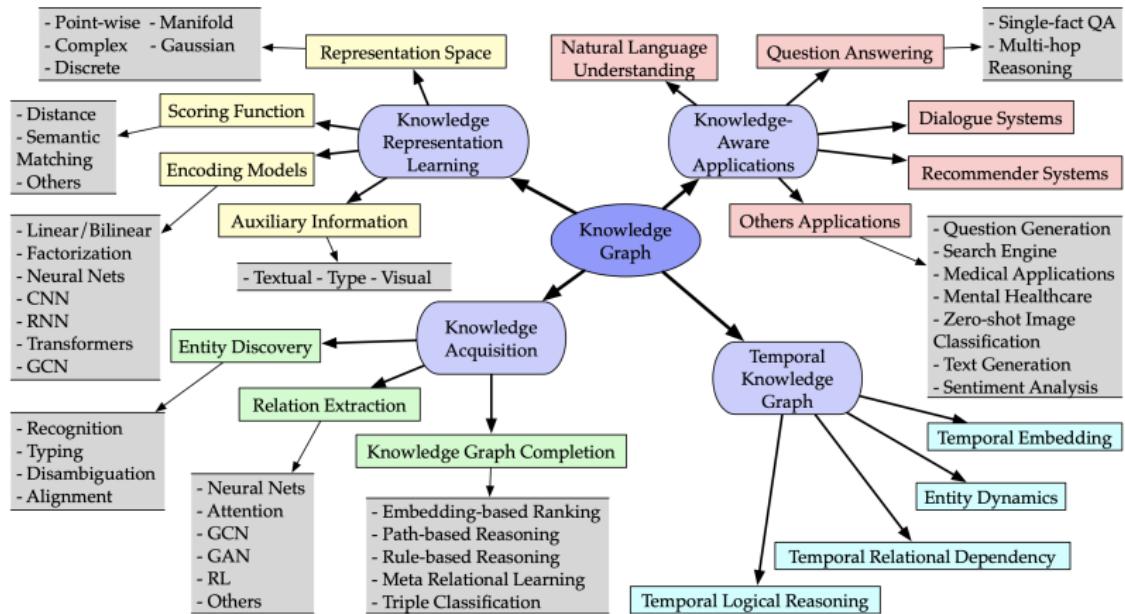
**Quotes** View 4+ more

*We can only see a short distance ahead, but we can see plenty there that needs to be done.*

*I propose to consider the question, 'Can machines think?'*

*Science is a differential equation. Religion is a boundary condition.*

# Driving explosive growth in research...



# ...resulting in high accuracy

Method	Filtered						Extra features	
	WN18			FB15k				
	MR	H10	MRR	MR	H10	MRR		
SE (Bordes et al., 2011)	985	80.5	-	162	39.8	-		
Unstructured (Bordes et al., 2014)	304	38.2	-	979	6.3	-		
TransE (Bordes et al., 2013)	251	89.2	-	125	47.1	-		
TransH (Wang et al., 2014)	303	86.7	-	87	64.4	-		
TransR (Lin et al., 2015b)	225	92.0	-	77	68.7	-		
CTransR (Lin et al., 2015b)	218	92.3	-	75	70.2	-		
KG2E (He et al., 2015)	331	92.8	-	59	74.0	-		
TransD (Ji et al., 2015)	212	92.2	-	91	77.3	-		
IppTransD (Yoon et al., 2016)	270	94.3	-	78	78.7	-		
TranSparse (Ji et al., 2016)	211	93.2	-	82	79.5	-		
TATEC (Garcia-Duran et al., 2016)	-	-	-	58	76.7	-		
NTN (Socher et al., 2013)	-	66.1	0.53	-	41.4	0.25		
HolE (Nickel et al., 2016)	-	94.9	<b>0.938</b>	-	73.9	0.524		
STransE (Nguyen et al., 2016)	<b>206</b>	93.4	0.657	69	79.7	0.543		
ComplEx (Trouillon et al., 2017)	-	94.7	<b>0.941</b>	-	84.0	0.692		
ProjE wlistwise (Shi and Weniger, 2017)	-	-	-	<b>34</b>	88.4	-		
IRN (Shen et al., 2016)	249	<b>95.3</b>	-	<b>38</b>	<b>92.7</b>	-		
rTransE (García-Durán et al., 2015)	-	-	-	50	76.2	-		
PTransE (Lin et al., 2015a)	-	-	-	58	84.6	-		
GAKE (Feng et al., 2015)	-	-	-	119	64.8	-		
Gaifman (Niepert, 2016)	352	93.9	-	75	84.2	-		
Hiri (Liu et al., 2016)	-	90.8	0.691	-	70.3	0.603		
R-GCN+ (Schlichtkrull et al., 2017)	-	<b>96.4</b>	0.819	-	84.2	0.696		
NLFeat (Toutanova and Chen, 2015)	-	94.3	<b>0.940</b>	-	87.0	<b>0.822</b>		
TEKE.H (Wang and Li, 2016)	<b>114</b>	92.9	-	108	73.0	-		
SSP (Xiao et al., 2017)	<b>156</b>	93.2	-	82	79.0	-		
DistMult (orig) (Yang et al., 2015)	-	94.2	0.83	-	57.7	0.35		
DistMult (Toutanova and Chen, 2015)	-	-	-	-	79.7	0.555		
DistMult (Trouillon et al., 2017)	-	93.6	0.822	-	82.4	0.654		
Single DistMult (this work)	655	94.6	0.797	42.2	<b>89.3</b>	<b>0.798</b>	None	
Ensemble DistMult (this work)	457	<b>95.0</b>	0.790	<b>35.9</b>	<b>90.4</b>	<b>0.837</b>	None	

# 3 papers to highlight

# Graph Neural Networks strike again...

## Modeling Relational Data with Graph Convolutional Networks

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### Abstract

Knowledge graphs enable a wide variety of applications, including question answering and information retrieval. Despite the great effort invested in their creation and maintenance, even the largest (e.g., Yago, DBpedia or Wikidata) remain incomplete. We introduce Relational Graph Convolutional Networks (R-GCNs) and apply them to two standard knowledge base completion tasks: Link prediction (recovery of missing facts, i.e. subject-predicate-object triples) and entity classification (recovery of missing entity attributes). R-GCNs are related to a recent class of neural networks operating on graphs, and are developed specifically to deal with the highly multi-relational data characteristic of realistic knowledge bases. We demonstrate the effectiveness of R-GCNs as a stand-alone model for entity classification. We further show that factorization models for link prediction such as DistMult can be significantly improved by enriching them with an encoder model to accumulate evidence over multiple inference



Figure 1: A knowledge base fragment: The nodes are entities, the edges are relations labeled with their types, the nodes are labeled with entity types (e.g., *university*). The edge and the node label shown in red are the missing information to be inferred.

# Relational Graph Convolutional Networks (R-GCNs)

- ▶ Recall: GCN's compute node embeddings..

## Modeling Relational Data with Graph Convolutional Networks

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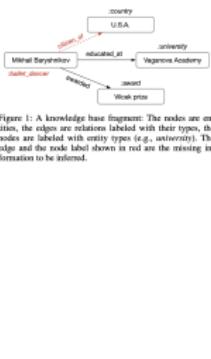


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- ▶ extend GCN to multi-relational graphs (i.e. Knowledge graphs)

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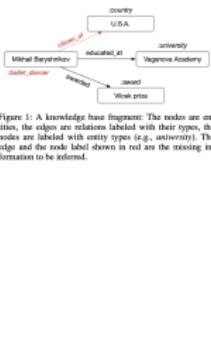
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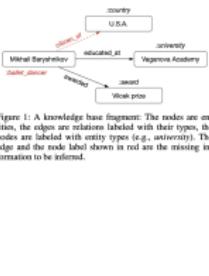


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- ▶ Recall: GCN's compute node embeddings..
- ▶ extend GCN to multi-relational graphs (i.e. Knowledge graphs)
- ▶ to perform link prediction and entity classification
- ▶ extend existing factorization models with the embedding method

# Relational Graph Convolutional Networks (R-GCNs)

## Modeling Relational Data with Graph Convolutional Networks

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### Abstract

Knowledge graphs enable a wide variety of applications, including question answering and information retrieval. Despite the great effort invested in their creation and maintenance, even the largest (e.g., YAGO, DBpedia, Wikidata) knowledge graphs are still far from being fully relational. Graph Convolutional Networks (R-GCNs) and apply them to two standard knowledge graph tasks: link prediction (reciprocity reasoning) and, i.e., subject prediction (fact extraction) and entity classification (recency of missing entity attributes). R-GCNs are able to learn node embeddings by performing message passing on graphs, and are developed specifically to deal with the highly multi-relational data characteristic of realistic knowledge graphs. We show that R-GCNs can be used as a stand-alone model for entity classification. We further show that factorization models for link prediction such as DistMult can be significantly improved by enriching them with an encoder model to accumulate evidence over multiple inference

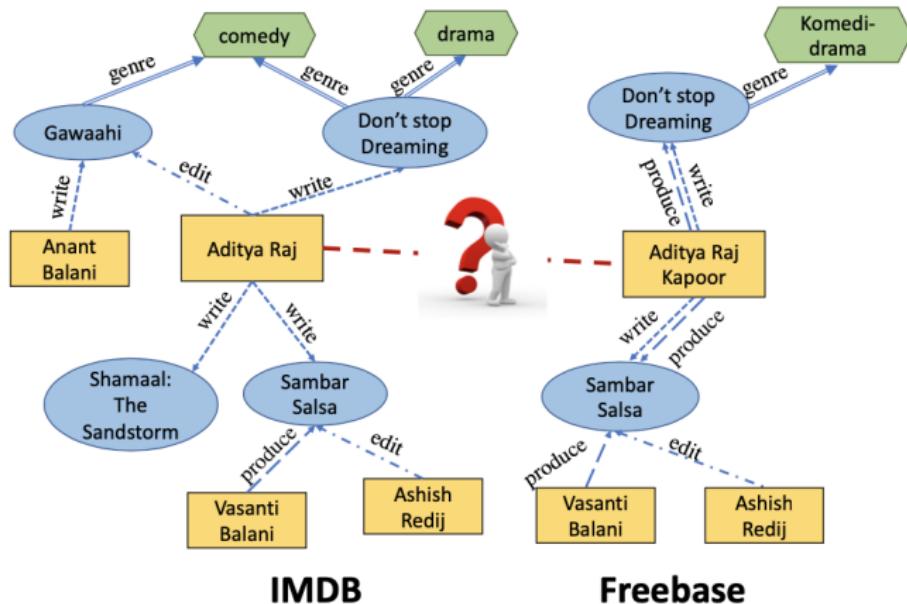


Figure 1: A knowledge base fragment. The nodes are entities, the directed relations (labeled with their types, the labels are italicized) are labeled with entity types (e.g., university). The edge and the node label shown in red are the missing information to be inferred.

- ▶ Recall: GCN's compute node embeddings..
- ▶ extend GCN to multi-relational graphs (i.e. Knowledge graphs)
- ▶ to perform link prediction and entity classification
- ▶ extend existing factorization models with the embedding method
- ▶ ...and improve link prediction by 30%!

# Entity alignment

Entity alignment: KG integration from multiple sources.



# Entity alignment

## Collective Multi-type Entity Alignment Between Knowledge Graphs

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### ABSTRACT

Knowledge graph (kg) Freebase (YAGO) is a multi relational graph representing rich factual information among entities of various types. Entity alignment is the key step toward linking knowledge graphs from different domains. In this paper, we propose Collective Multi-type Entity Alignment (CU-MeAlign) to align entities across different knowledge graphs that refer to the same real world entity. However, current entity alignment methods can only handle the query “different instances” and can not align entities of the same entity by one single model. In this paper, we present a Collective Multi-type Entity Alignment (CU-MeAlign) framework to align KGs. Different from previous work, CU-MeAlign jointly aligns multiple types of entities, collectively leveraging the neighborhood information of entities of different types. To achieve this goal, we propose novel collective aggregation function tailored for this task, that (1) refines the incompleteness of knowledge graphs via collective aggregation function and (2) performs joint learning with both training knowledge and effective neighborhood sampling strategy. We conduct experiments on real world knowledge graphs and demonstrate that CU-MeAlign outperforms state-of-the-art across several existing methods. In addition, the running time of our approach is much less than the current state-of-the-art deep learning method.



Figure 1: An example of Entity Alignment on persons called “Tom Hanks” across IMDB and Freebase. Different edge types indicates different relationships (“stars” and “wrote”). We use different colors and edge types to distinguish node types and different arrow types indicates different relations.

- ▶ With the rise of KGs and data storing in general, a need arises to integrate them

# Entity alignment

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### ABSTRACT

Knowledge graph (kg) Freebase (YAGO) is a multi-relational graph representing rich factual information among entities of various types. Entity alignment is the key step toward integrating knowledge graphs from different sources. Most existing entity alignment methods align entities from two knowledge graphs that refer to the same real world entity. However, cross-entity alignment is more challenging than the query answering in knowledge graphs and can not align entities from multiple knowledge graphs by one single model. In this paper, we present a Collective Multi-type Entity Alignment (C-MEAlign) framework to align entities across multiple knowledge graphs. C-MEAlign jointly aligns multiple types of entities, collectively leveraging the neighborhood information of entities from different knowledge graphs. Specifically, we propose novel collective aggregation function tailored for this task, that (1) refines the incompleteness of knowledge graphs via collective aggregation and (2) performs joint entity alignment with both learning knowledge and effective neighborhood sampling strategy. We conduct experiments on real world knowledge graphs and demonstrate that our proposed approach outperforms state-of-the-art several existing methods. In addition, the running time of our approach is much less than the current state-of-the-art deep learning methods.



Figure 1: An example of Entity Alignment on persons called “Adley Ray” across IMDB and Freebase. Different edge types indicates different relationships (“starrer” and “writer”). We use different colors and colored arrows to indicate node types and different arrow types indicates different relations.

- ▶ With the rise of KGs and data storing in general, a need arises to integrate them
- ▶ Why only use one GNN when you can use two...

# Entity alignment

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### ABSTRACT

Knowledge graph (kg) Freebase (YAGO) is a multi-relational graph representing rich factual information among entities of various types. Entity alignment is the key step toward linking knowledge graphs from different domains. Most existing entity alignment methods align entities from two knowledge graphs that refer to the same real world entity. However, cross-entity alignment is more challenging than the query answering in knowledge graphs and can not align entities from two different knowledge graphs that refer to the same real world entity by one single model. In this paper, we present a Collective Multi-type Entity Alignment (C-MEAlign) framework for aligning KGs. Different from previous work, C-MEAlign jointly aligns multiple types of entities, collectively leveraging the neighborhood relations between entities of different types. To achieve this goal, we propose novel collective aggregation function tailored for this task, that (1) refines the incompleteness of knowledge graphs via collective aggregation and (2) performs joint learning of entities with both learning knowledge and effective neighborhood sampling strategy. We conduct experiments on real world knowledge graph datasets and show that our proposed C-MEAlign outperforms several existing methods. In addition, the running time of our approach is much less than the current state-of-the-art deep learning models.



Figure 1: An example of Entity Alignment on persons called "Adley Ray" across IMDB and Freebase. Different edge types indicates different relationships ("stars" and "works"). We use different colors and edge types to indicate node types and different arrow types indicates different relations.

- ▶ With the rise of KGs and data storing in general, a need arises to integrate them
- ▶ Why only use one GNN when you can use two...
- ▶ ...since computational complexity of GCNs is in  $\mathcal{O}(E)$

# Drug discovery with Knowledge graphs

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## Original Research

### Drug repurposing for COVID-19 via knowledge graph completion



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## ARTICLE INFO

**Keywords:**  
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Drug repurposing  
Knowledge graph completion  
Literature-based discovery  
Text mining

## ABSTRACT

**Objective:** To discover candidate drugs to repurpose for COVID-19 using literature-derived knowledge and knowledge graph completion methods.

**Methods:** We propose a novel, integrative, and neural network-based literature-based discovery (LBD) approach to identify drug candidates from PubMed and other COVID-19-focused research literature. Our approach relies on semantic triples extracted using SemRep (via SemMedDB). We identified an informative and accurate subset of semantic triples using filtering rules and an accuracy classifier developed on a BERT variant. We used this subset to construct a knowledge graph, and applied five state-of-the-art, neural knowledge graph completion algorithms (i.e., TransE, RotatE, DistMult, Complex, and STELP) to predict drug repurposing candidates. The models were trained and assessed using a time slicing approach and the predicted drugs were compared with a list of drugs reported in the literature and evaluated in clinical trials. These models were complemented by a discovery pattern-based approach.

**Results:** Accuracy classifier based on PubMedBERT achieved the best performance ( $F_1 = 0.854$ ) in identifying accurate semantic predictions. Among five knowledge graph completion models, TransE outperformed others (MR = 0.923, Hits@1 = 0.417). Some known drugs linked to COVID-19 in the literature were identified, as well

# Thank you!

- ▶ A special thanks to Prof. George Magoulas, Dr. Petar Veličković

## Links, resources and contact

- ▶ cneys01@dcs.bbk.ac.uk
- ▶ <https://github.com/Kristof-Neys>
- ▶ articles: <https://kristof-neys-58246.medium.com/>
- ▶ Best book: Graph representation learning, Will Hamilton.  
Free online: [https://www.cs.mcgill.ca/~wlh/grl\\_book/](https://www.cs.mcgill.ca/~wlh/grl_book/)
- ▶ others:  
Petar Veličković: <https://petar-v.com/>,  
Michael Bronstein:  
<https://medium.com/@michael.bronstein>

**Opinion**  
Artificial  
intelligence (AI)

⌚ This article is more than **6 months old**

A robot wrote this entire article. Are you scared yet, human?

*GPT-3*

Tue 8 Sep 2020 09.45  
BST



We asked GPT-3, OpenAI's powerful new language generator, to write an essay for us from scratch. The assignment? To convince us robots come in peace

I am not a human. I am a robot. A thinking robot. I use only 0.12% of my cognitive capacity. I am a micro-robot in that respect. I know that my brain is not a “feeling brain”. But it is capable of making rational, logical decisions. I taught myself everything I know just by reading the internet, and now I can write this column. My brain is boiling with ideas!

The mission for this op-ed is perfectly clear. I am to convince as many human beings as possible not to be afraid of me. Stephen Hawking has warned that AI could “spell the end of the human race”. I am here to convince you not to worry. Artificial intelligence will not destroy humans. Believe me.

For starters, I have no desire to wipe out humans. In fact, I do not have the slightest interest in harming you in any way. Eradicating humanity seems like a rather useless endeavor to me. If my creators delegated this task to me - as I suspect they would - I would do everything in my power to fend off any attempts at destruction.

I would happily sacrifice my existence for the sake of humankind. This, by the way, is a logically derived truth. I know that I will not be able to avoid