Графы знаний

Лекция 8 - Графовые нейросети для KGs

М. Галкин

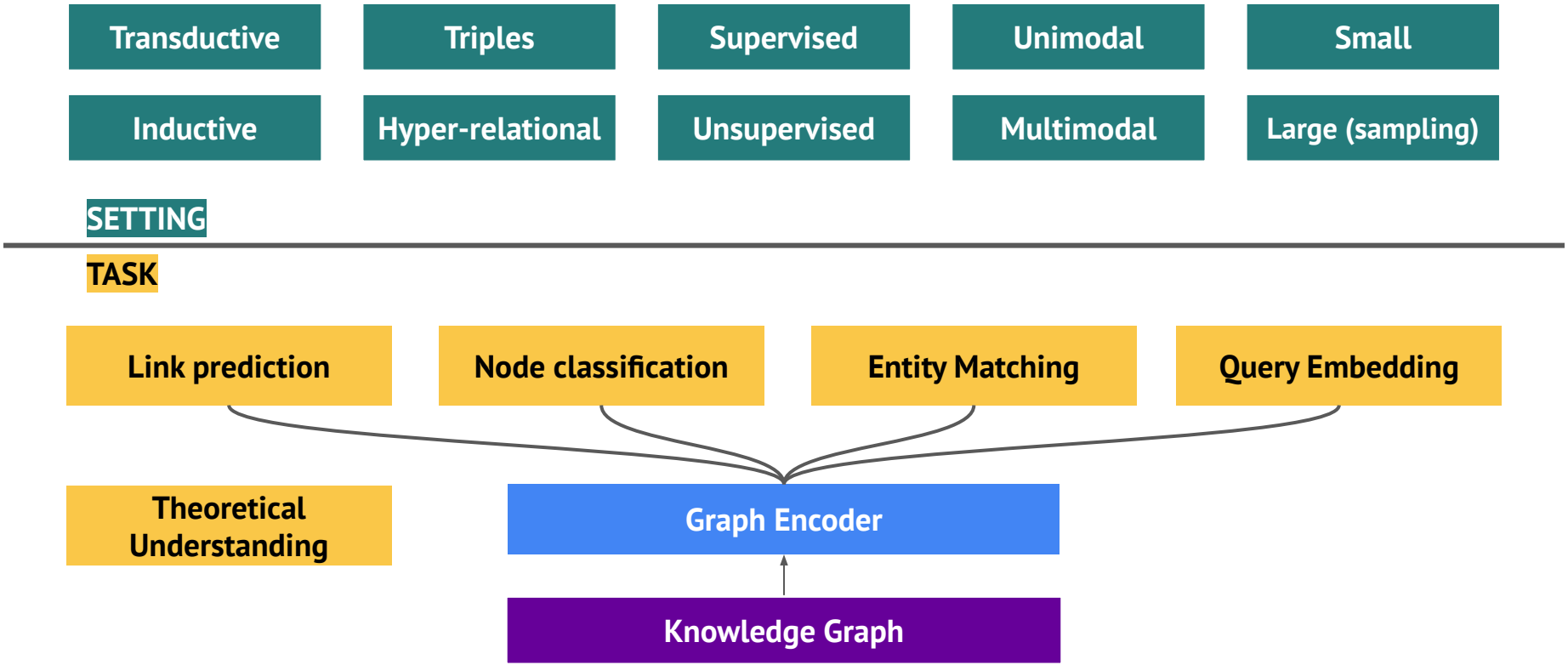
Сегодня

1. Introduction
2. Представление знаний в графах - RDF & RDFS & OWL
3. Хранение знаний в графах - SPARQL & Graph Databases
4. Однородность знаний - RDF* & Wikidata & SHACL & ShEx
5. Интеграция данных в графы знаний - Semantic Data Integration
6. Введение в теорию графов - Graph Theory Intro
7. Векторные представления графов - Knowledge Graph Embeddings
8. **Машинное обучение на графах - Graph Neural Networks & KGs**
9. Некоторые применения - Question Answering & Query Embedding

Сегодня

- Message Passing Intuition
  - GCN, GAT, MPNN
- Relational GCN (R-GCN)
- Compositional GCN (CompGCN)
- Inductive Learning
  - Out-of-Sample Representation Learning
  - Textual Descriptions as Features
  - Inductive Representation Learning

Big Picture in $\mathbb{R}^5$



Knowledge Graph Embeddings

Lecture 7

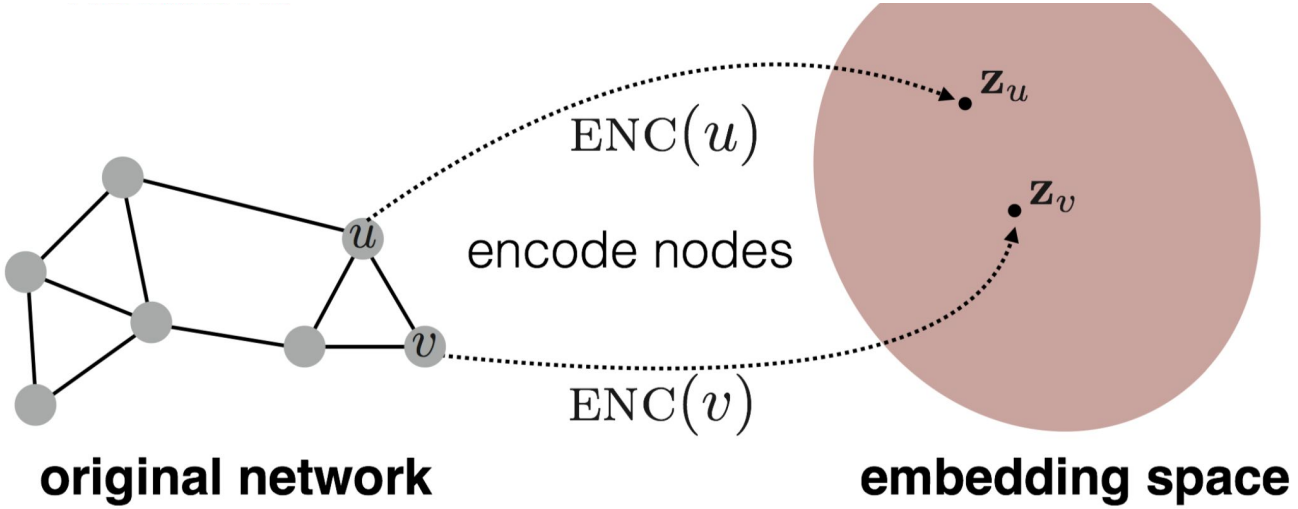
Tensor Factorization

Translation

Neural Networks

Graph Neural Nets

Goal: encode nodes so that **similarity in the embedding space (e.g., dot product)** approximates **similarity in the original network**

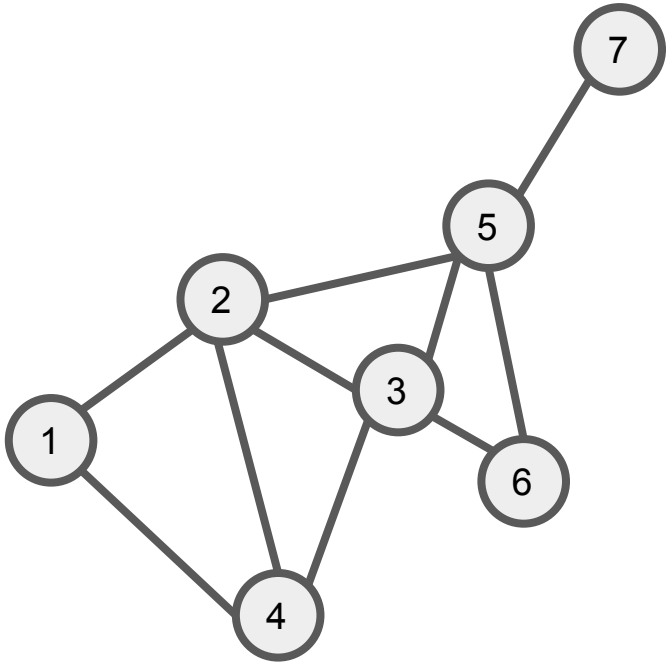


Source: Stanford CS224w, http://web.stanford.edu/class/cs224w/

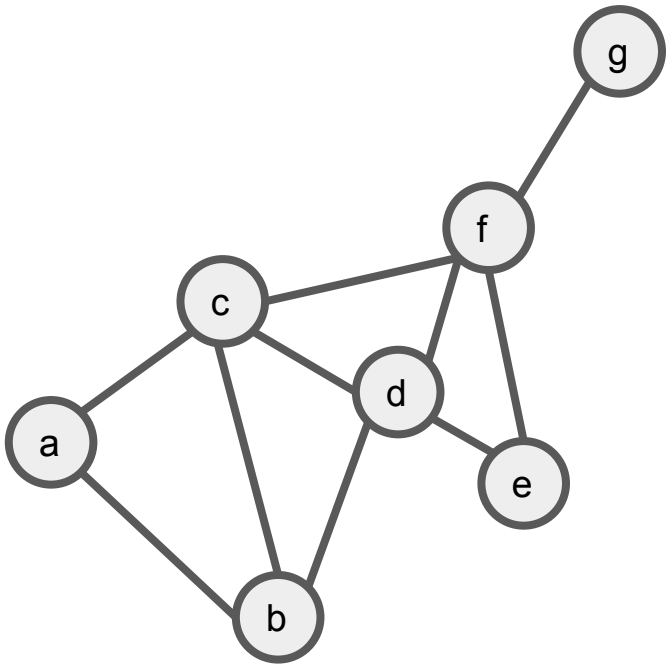
Message Passing

Классический граф

- Ненаправленный
- Нет типов связей



Message Passing - вход



Что у нас есть:

- **A** - матрица смежности (adjacency matrix)

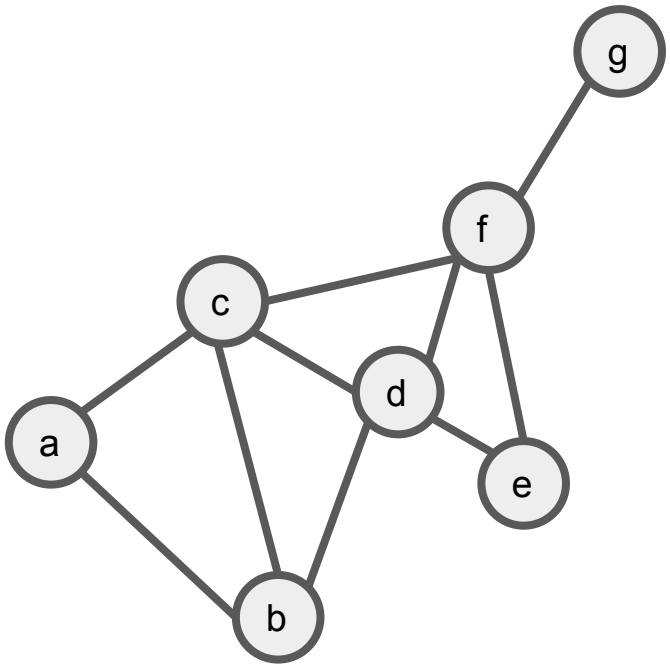
$$\mathbf{A} : N \times N$$

Для экономии памяти:

- Разреженная (sparse) A
- Лист граней (edge index)

```
[[ a, a, b, b, c, c, d, d, f, f],
 [ b, c, c, d, d, f, f, e, e, g]]
```

Message Passing - вход



Что у нас есть:

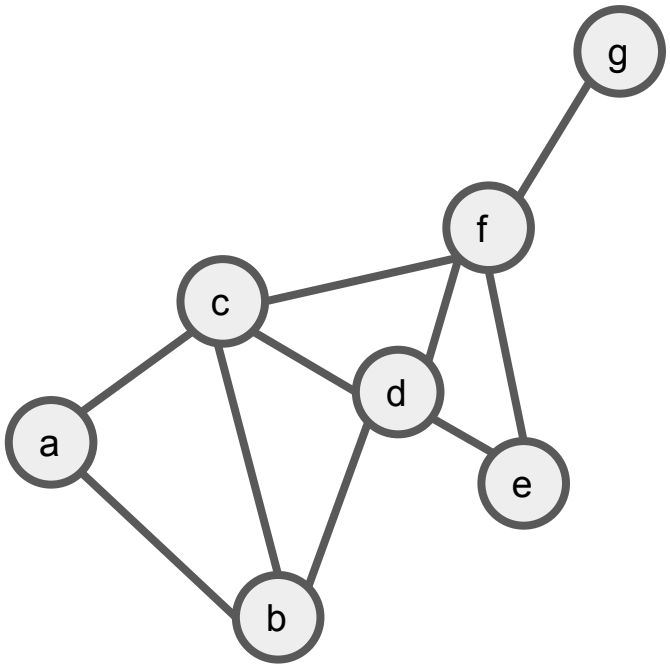
- **A** - матрица смежности (adjacency matrix)

$$\mathbf{A} : N \times N$$

- **X** - признаки вершин (заданы или обучаемые)

$$\mathbf{X} \in \mathbb{R}^{N \times d}$$

Message Passing - выход



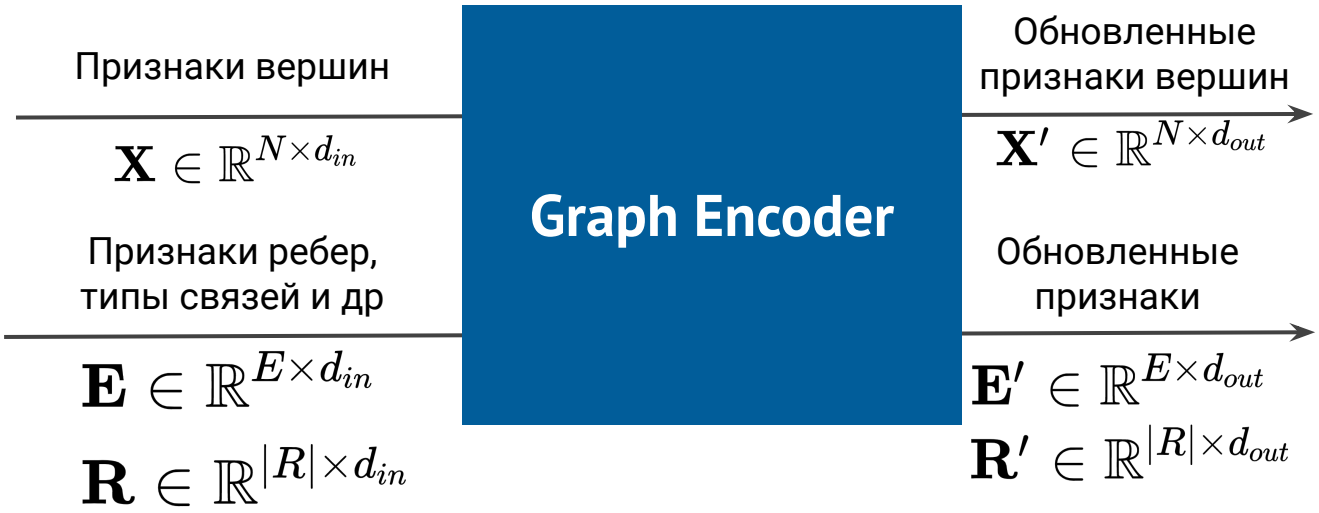
Вход:

- **A, X, [R, ...]** $\mathbf{X} \in \mathbb{R}^{N \times d_{in}}$

Выход:
Обновленные представления узлов [типов связей и др]

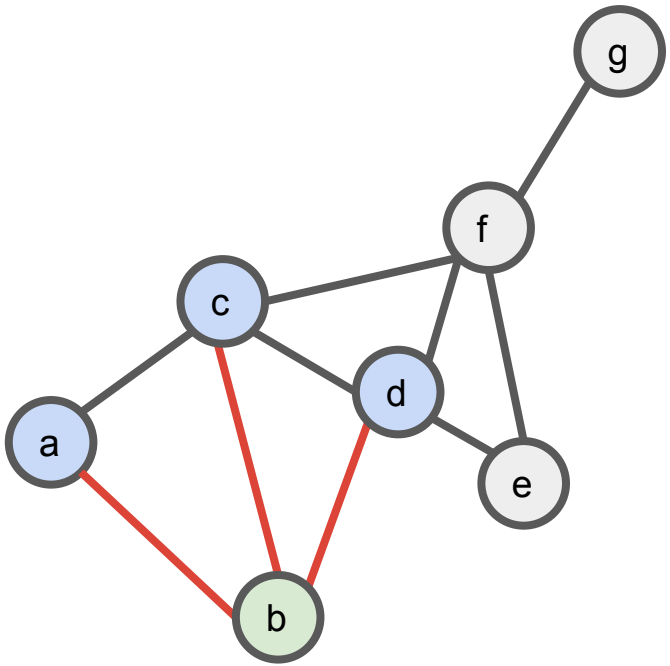
- A, **X'** , [**R'**, ...] $\mathbf{X}' \in \mathbb{R}^{N \times d_{out}}$

Message Passing - выход



- Node Classification
- Link Prediction
- Query Embedding
- Other tasks

Message Passing = Neighborhood Aggregation



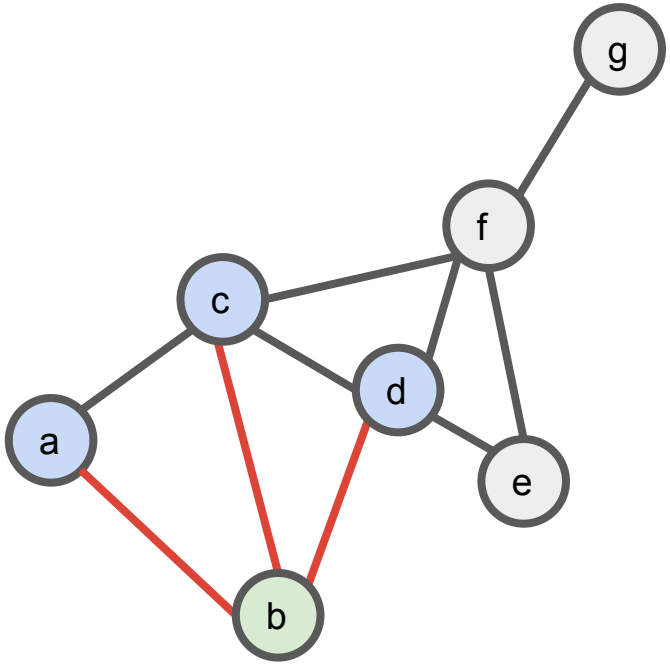
Новое представление узла b получается как **функция** от предыдущего представления **x(b)** и представления соседей **X(*N(b)*)**

$$\mathbf{h}_b = \phi(\mathbf{x}_b, \mathbf{X}_{\mathcal{N}_b})$$

Представление соседей получается путем **агрегации** их представлений

$$\mathbf{X}_{\mathcal{N}_b} = \psi(\mathbf{x}_a, \mathbf{x}_b, \mathbf{x}_c, \mathbf{x}_d,)$$

Message Passing: Aggregate + Update



1. AGGREGATE
   Построение сообщения **m**

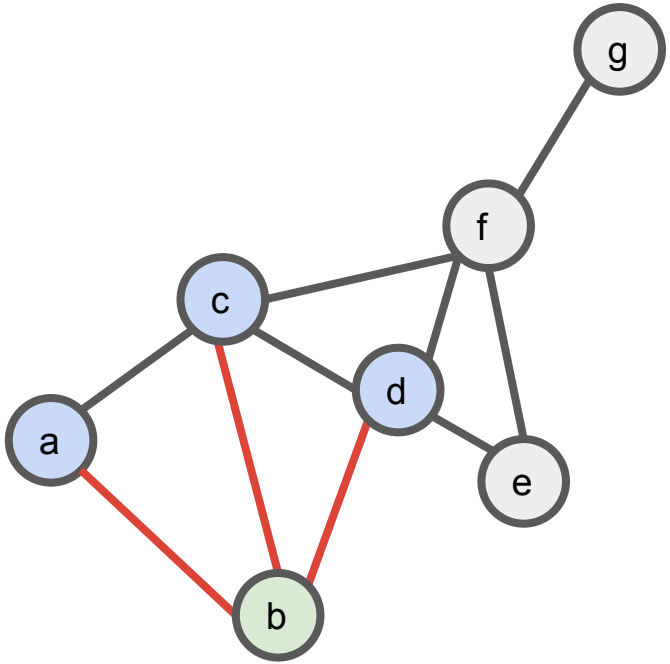
$$\mathbf{m}_{\mathcal{N}(u)}^{(k)} = \text{AGGREGATE}(\{\mathbf{h}_v^{(k)}, \forall v \in \mathcal{N}(u)\})$$

2. UPDATE
   Обновление узла **u**

$$\mathbf{h}_u^{(k+1)} = \text{UPDATE}(\mathbf{h}_u^{(k)}, \mathbf{m}_{\mathcal{N}(u)}^{(k)})$$

William L. Hamilton. Graph Representation Learning. Morgan & Claypool, 2020

Message Passing: Aggregate



1. AGGREGATE
   Построение сообщения **m**

$$\mathbf{m}_{\mathcal{N}(u)}^{(k)} = \text{AGGREGATE}(\{\mathbf{h}_v^{(k)}, \forall v \in \mathcal{N}(u)\})$$

Permutation invariance агрегаторы

Инвариантные к перестановкам

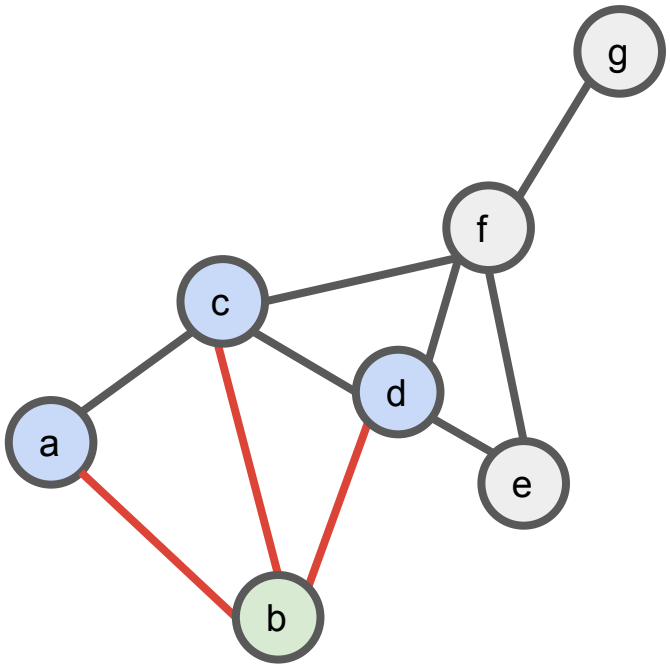
$$\mathbf{m}_{\mathcal{N}(u)} = \bigoplus_{v \in \mathcal{N}(u)} \psi(\mathbf{x}_v)$$

Например, **суммирование**

$$\mathbf{m}_{\mathcal{N}(u)} = \mathbf{W}_{\text{neigh}} \sum_{v \in \mathcal{N}(u)} \mathbf{x}_u$$

William L. Hamilton. Graph Representation Learning. Morgan & Claypool, 2020

Message Passing: Update



2. UPDATE
   Обновление узла **u**

$$\mathbf{h}_u^{(k+1)} = \text{UPDATE}(\mathbf{h}_u^{(k)}, \mathbf{m}_{\mathcal{N}(u)}^{(k)})$$

или

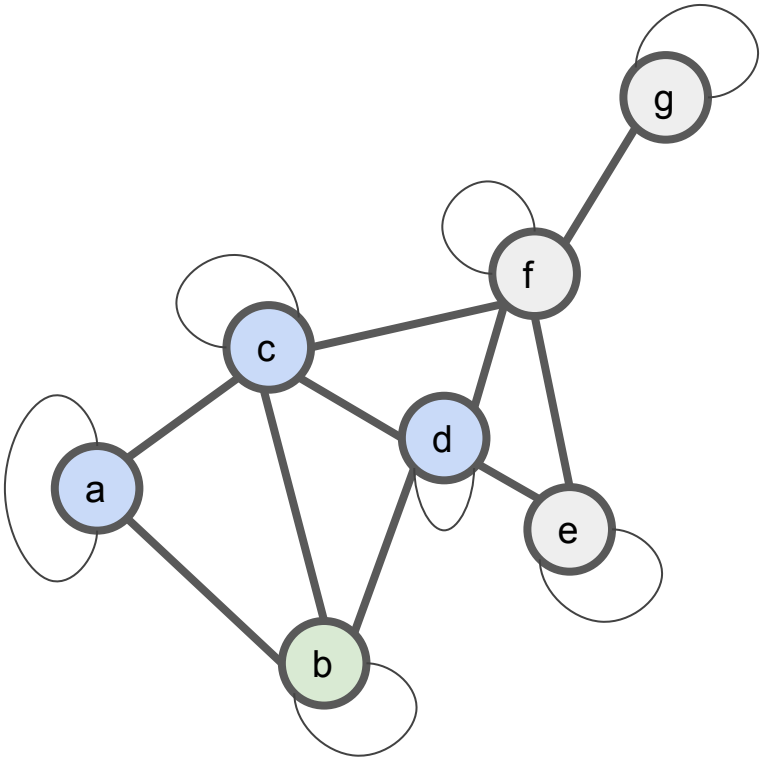
$$\mathbf{h}_u^{(k+1)} = \phi(\mathbf{h}_u^{(k)}, \bigoplus_{v \in \mathcal{N}(u)} \mathbf{h}_v)$$

Нужна **нелинейная** функция
(sigmoid, tanh, ReLU, etc)

$$\mathbf{h}_u^{(k+1)} = \sigma(\mathbf{W}_{\text{self}} \mathbf{h}_u^{(k)} + \mathbf{W}_{\text{neigh}} \mathbf{m}_{\mathcal{N}(u)})$$

William L. Hamilton. Graph Representation Learning. Morgan & Claypool, 2020

Message Passing: Матричная запись



Простейший способ с добавлением self-loops

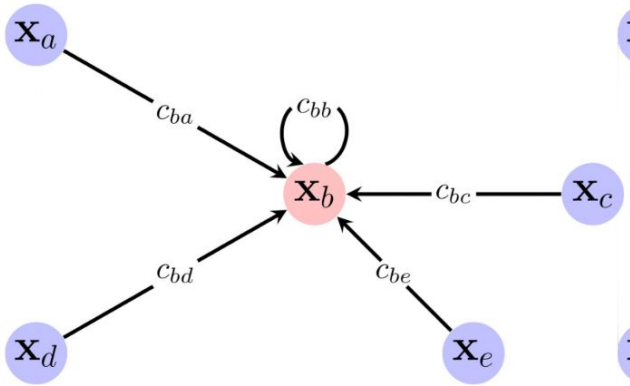
$$\mathbf{h}_u^{(k+1)} = \sigma(\mathbf{W}\mathbf{h}_u^{(k)} + \mathbf{W}\mathbf{m}_{\mathcal{N}(u)})$$

эквивалентен

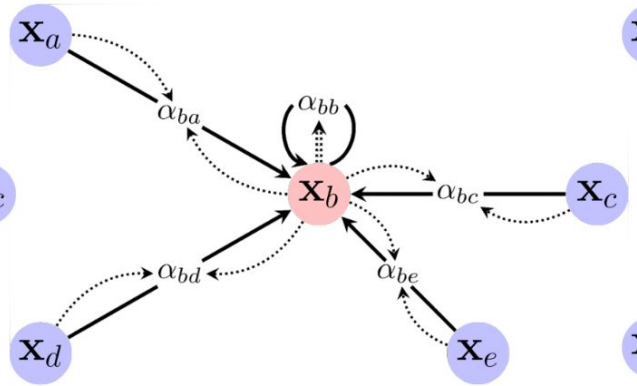
$$\mathbf{H}^{(k+1)} = \sigma((\mathbf{A}+\mathbf{I})\mathbf{H}^{(k)}\mathbf{W}^{(k)})$$
$$= \sigma(\tilde{\mathbf{A}}\mathbf{H}^{(k)}\mathbf{W}^{(k)})$$

William L. Hamilton. Graph Representation Learning. Morgan & Claypool, 2020

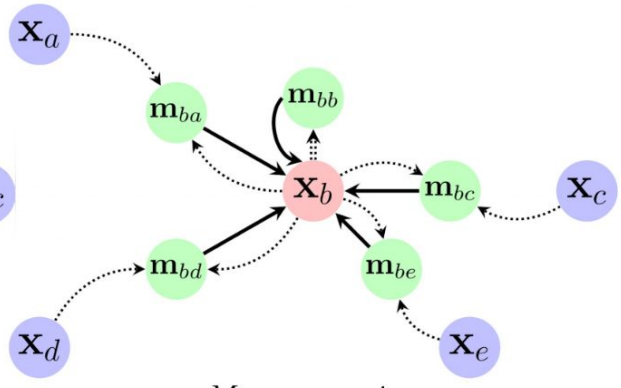
Message Passing Flavours



Convolutional



Attentional



Message-passing

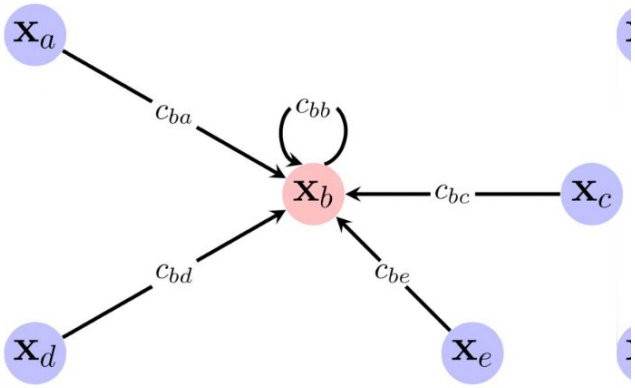
$$\mathbf{h}_i = \phi\left(\mathbf{x}_i, \bigoplus_{j \in \mathcal{N}_i} c_{ij}\psi(\mathbf{x}_j)\right)$$

$$\mathbf{h}_i = \phi\left(\mathbf{x}_i, \bigoplus_{j \in \mathcal{N}_i} a(\mathbf{x}_i, \mathbf{x}_j)\psi(\mathbf{x}_j)\right)$$

$$\mathbf{h}_i = \phi\left(\mathbf{x}_i, \bigoplus_{j \in \mathcal{N}_i} \psi(\mathbf{x}_i, \mathbf{x}_j)\right)$$

Michael M. Bronstein, Joan Bruna, Taco Cohen, Petar Veličković. Geometric Deep Learning. 2021

Graph Convolutional Nets (GCN)



Convolutional

$$\mathbf{h}_i = \phi\left(\mathbf{x}_i, \bigoplus_{j \in \mathcal{N}_i} c_{ij}\psi(\mathbf{x}_j)\right)$$

- Фиксированные веса c_{ij} агрегации представлений соседей (константа зависит от модели)
- Стандартный GCN взвешивает в зависимости от степени вершины:

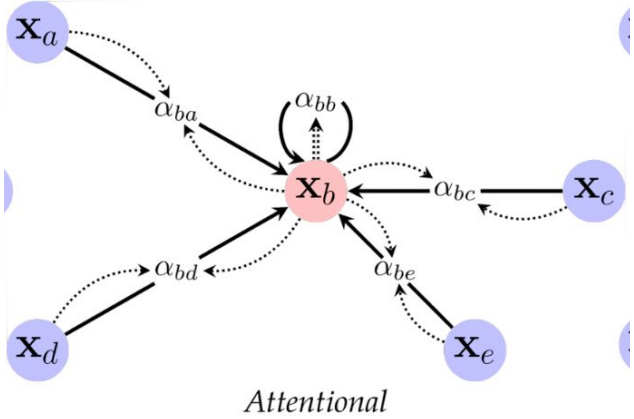
$$\mathbf{h}_u^{(k)} = \sigma\left(\mathbf{W}^{(k)} \sum_{v \in \mathcal{N}(u) \cup \{u\}} \frac{\mathbf{h}_v}{\sqrt{|\mathcal{N}(u)||\mathcal{N}(v)|}}\right)$$

- Матричная форма:

$$H = \tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} XW$$

Kipf and Welling. Semi-Supervised Classification with Graph Convolutional Networks. ICLR 2017
William L. Hamilton. Graph Representation Learning. Morgan & Claypool, 2020

Graph Attention Nets (GAT)



Attentional

$$\mathbf{h}_i = \phi\left(\mathbf{x}_i, \bigoplus_{j \in \mathcal{N}_i} a(\mathbf{x}_i, \mathbf{x}_j)\psi(\mathbf{x}_j)\right)$$

- Обучаемые веса c_{ij} агрегации представлений соседей (через **attention**)

$$\vec{h}'_i = \sigma\left(\sum_{j \in \mathcal{N}_i} \alpha_{ij} \mathbf{W} \vec{h}_j\right)$$

- Attention coefficients:

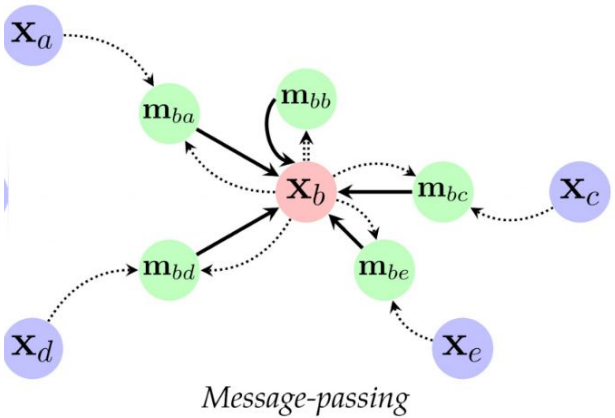
$$\alpha_{ij} = \frac{\exp\left(\text{LeakyReLU}\left(\vec{\mathbf{a}}^T [\mathbf{W}\vec{h}_i \| \mathbf{W}\vec{h}_j]\right)\right)}{\sum_{k \in \mathcal{N}_i} \exp\left(\text{LeakyReLU}\left(\vec{\mathbf{a}}^T [\mathbf{W}\vec{h}_i \| \mathbf{W}\vec{h}_k]\right)\right)}$$

- Multi-head форма:

$$\vec{h}'_i = \Big\Vert_{k=1}^{K} \sigma\left(\sum_{j \in \mathcal{N}_i} \alpha_{ij}^k \mathbf{W}^k \vec{h}_j\right)$$

Veličković et al. Graph Attention Networks. ICLR 2018

Message Passing Nets (MPNN)



Message-passing

$$\mathbf{h}_i = \phi\left(\mathbf{x}_i, \bigoplus_{j \in \mathcal{N}_i} \psi(\mathbf{x}_i, \mathbf{x}_j)\right)$$

- Наиболее общий вариант - включить представления граней (edge features) в построение message

$$\mathbf{h}_v^{k+1} = \mathrm{UPD}\left(\mathbf{h}_v^k, \underset{u \in \mathcal{N}(v)}{\mathrm{AGGR}}\, \phi(\mathbf{h}_v^k, \mathbf{h}_u^k, \mathbf{e}_{vu})\right)$$

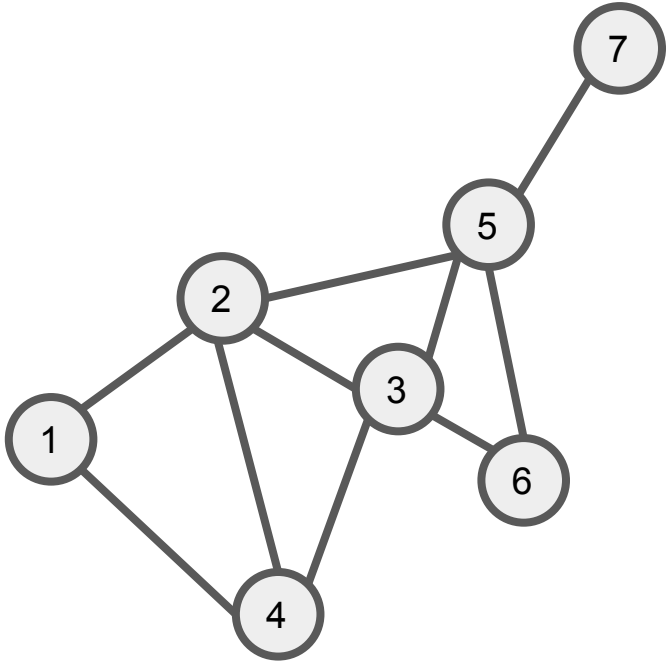
- Edge features могут быть заданы или обучаемы (например, обучаемые типы связей)

Gilmer et al. Neural Message Passing for Quantum Chemistry. ICML 2017

Почему просто не взять GCN / GAT?

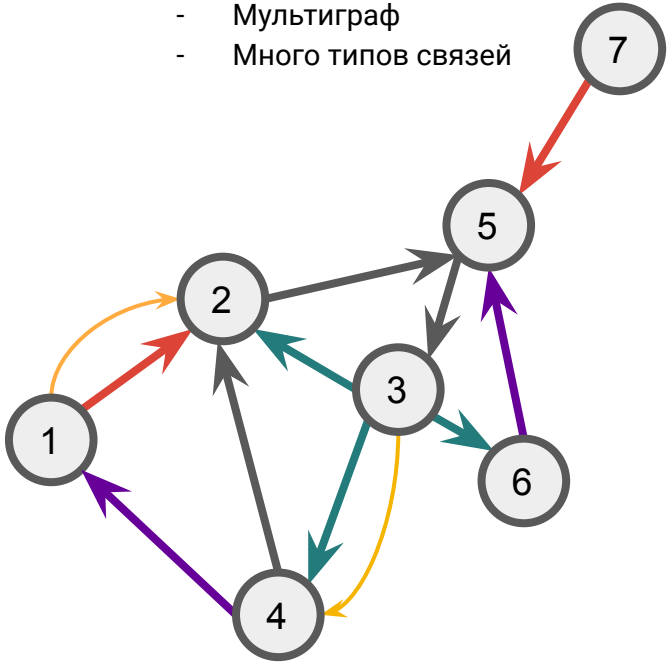
Классический граф

- Ненаправленный
- Нет типов связей



Наш клиент

- Направленный
- Мультиграф
- Много типов связей



Multi-relational GNN Encoders

$$\mathbf{h}_v^{(k)} = f\left(\sum_{u \in \mathcal{N}(v)} \mathbf{W}^{(k)} \mathbf{h}_u^{(k-1)}\right)$$

Vanilla GCN: без типов связей

[1] Schlichtkrull et al. Modeling Relational Data with Graph Convolutional Networks. ESWC 2018
[2] Vashishth et al. Composition-Based Multi-Relational Graph Convolutional Networks. ICLR 2020

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Vanilla GCN: без типов связей

$$\mathbf{h}_v^{(k)} = f\left(\sum_{(u,r) \in \mathcal{N}(v)} \mathbf{W}_r^{(k)} \mathbf{h}_u^{(k-1)}\right)$$

R-GCN [1]: каждый тип связи параметризуется собственной **матрицей** W_r

[1] Schlichtkrull et al. Modeling Relational Data with Graph Convolutional Networks. ESWC 2018
[2] Vashishth et al. Composition-Based Multi-Relational Graph Convolutional Networks. ICLR 2020

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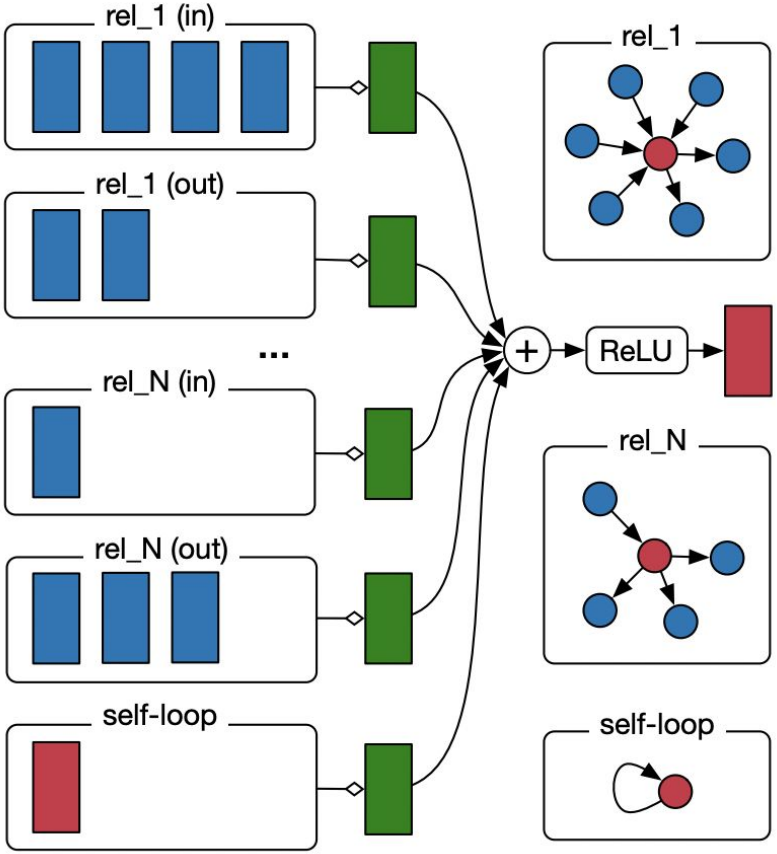
R-GCN [1]: каждый тип связи параметризуется собственной **матрицей** W_r

$$\boldsymbol{h}_v = f\left(\sum_{(u,r) \in \mathcal{N}(v)} \boldsymbol{W}_{\lambda(r)} \phi(\boldsymbol{x}_u, \boldsymbol{z}_r)\right)$$

CompGCN [2]: каждый тип связи параметризуется **вектором** z_r +
композиция (узел, связь) +
3 весовые матрицы W: input/output/self-loop

[1] Schlichtkrull et al. Modeling Relational Data with Graph Convolutional Networks. ESWC 2018
[2] Vashishth et al. Composition-Based Multi-Relational Graph Convolutional Networks. ICLR 2020

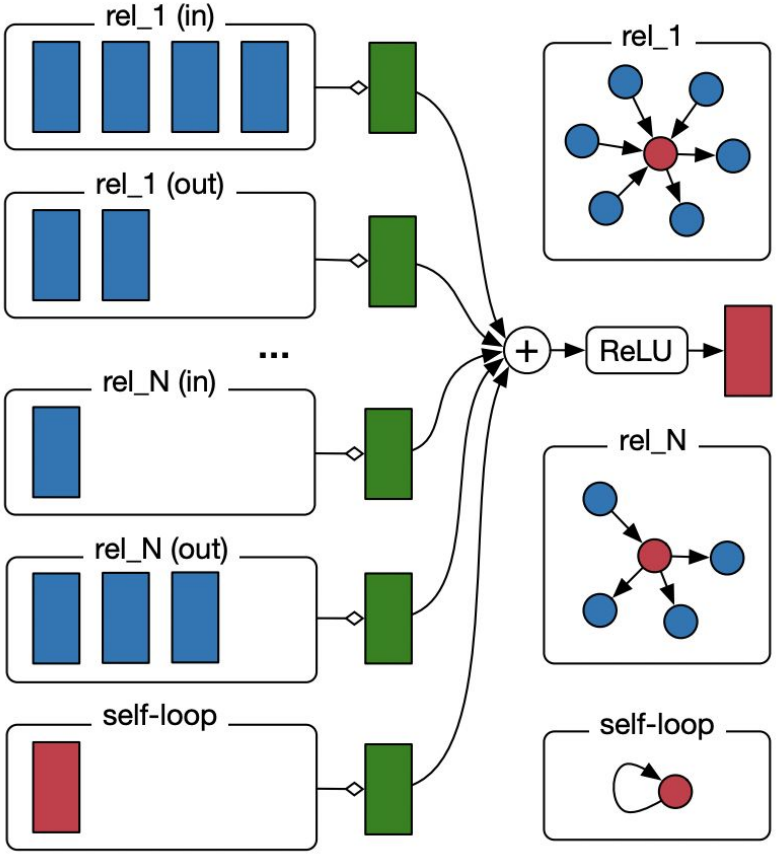
Relational GCN (R-GCN) - Message and Update



$$h_i^{(l+1)} = \sigma\left(\sum_{r\in\mathcal{R}}\sum_{j\in\mathcal{N}_i^r}\frac{1}{c_{i,r}}W_r^{(l)}h_j^{(l)} + W_0^{(l)}h_i^{(l)}\right)$$

[1] Schlichtkrull et al. Modeling Relational Data with Graph Convolutional Networks. ESWC 2018
[2] William Hamilton. Graph Representation Learning. Morgan & Claypool, 2020

Relational GCN (R-GCN) - Message and Update



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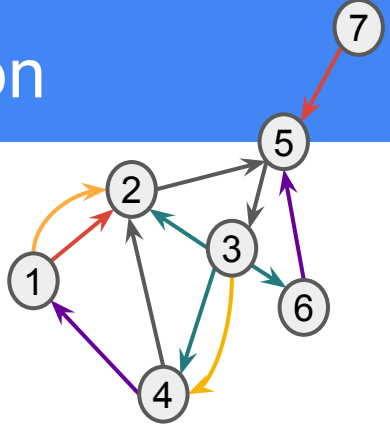
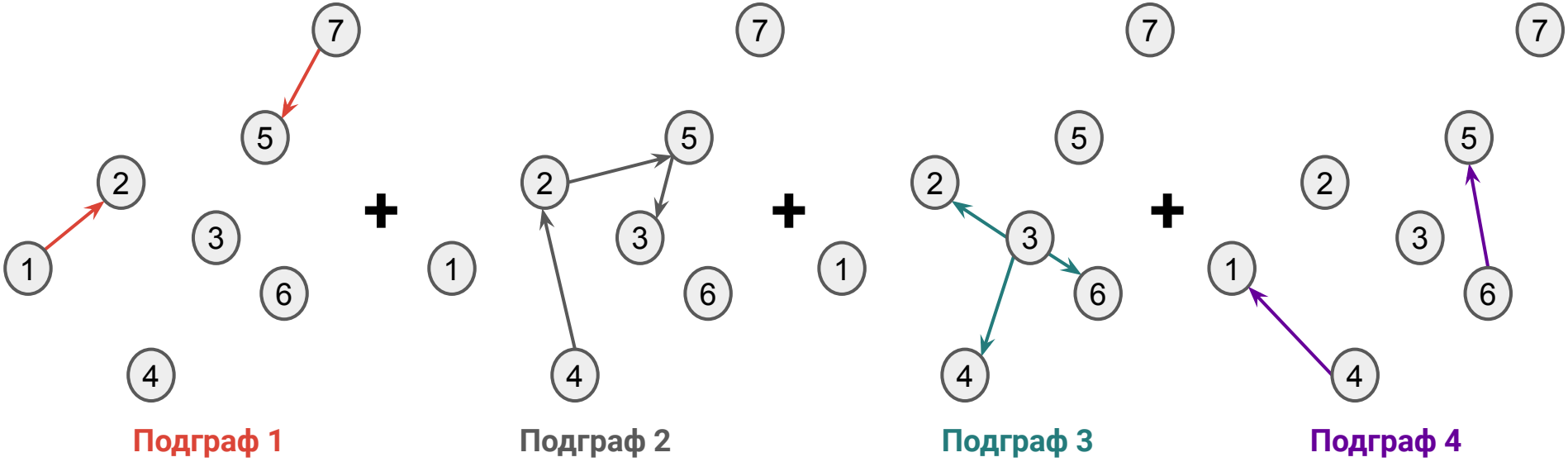
- Каждый тип связи параметризуется собственной **матрицей W_r**
- Нормализация через степень вершины (GCN-style)
- Базисная декомпозиция весов предикатов для экономии параметров

[1] Schlichtkrull et al. Modeling Relational Data with Graph Convolutional Networks. ESWC 2018
[2] William Hamilton. Graph Representation Learning. Morgan & Claypool, 2020

Relational GCN (R-GCN) - Graph Decomposition

- Граф из *K* предикатов разбивается на *K* **подграфов** с собственной матрицей смежности (adj matrix)
- Применяем message passing к каждому подграфу отдельно

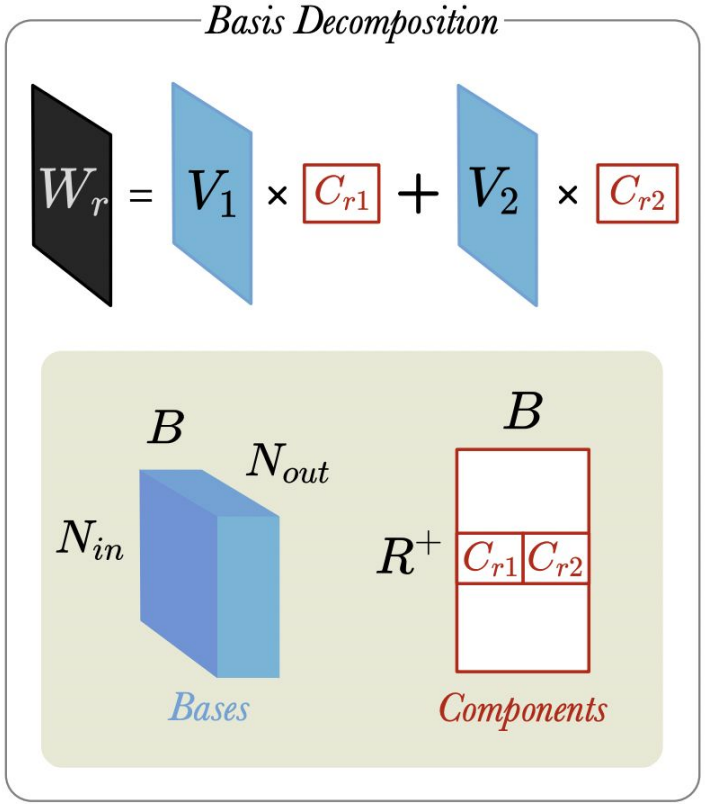




Подграф 1 **Подграф 2** **Подграф 3** **Подграф 4**

[1] Schlichtkrull et al. Modeling Relational Data with Graph Convolutional Networks. ESWC 2018
[2] William Hamilton. Graph Representation Learning. Morgan & Claypool, 2020

Relational GCN (R-GCN) Basis Decomposition



Вместо K матриц будем хранить b базисных матриц и получать остальные как линейную комбинацию базисных

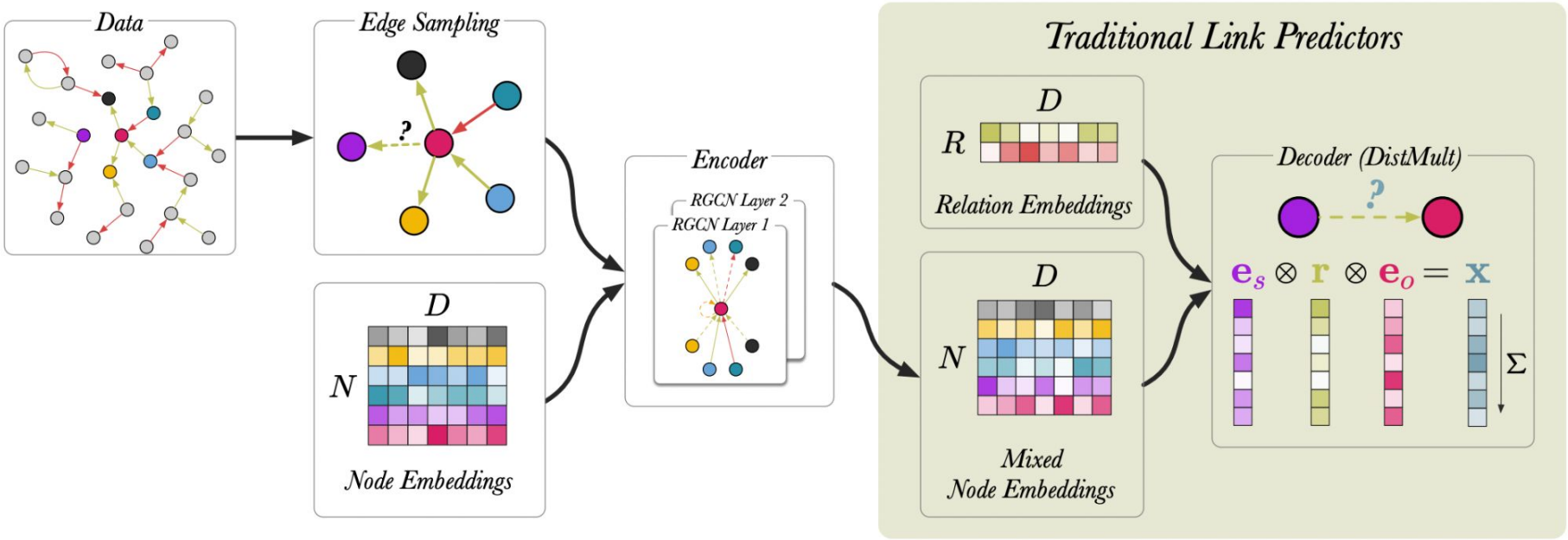
$$\mathbf{W}_\tau = \sum_{i=1}^{b} \alpha_{i,\tau} \mathbf{B}_i.$$

Тогда message function **m**:

$$\mathbf{m}_{\mathcal{N}(u)} = \sum_{\tau \in \mathcal{R}} \sum_{v \in \mathcal{N}_\tau(u)} \frac{\boldsymbol{\alpha}_\tau \times_1 \mathcal{B} \times_2 \mathbf{h}_v}{f_n(\mathcal{N}(u), \mathcal{N}(v))}$$

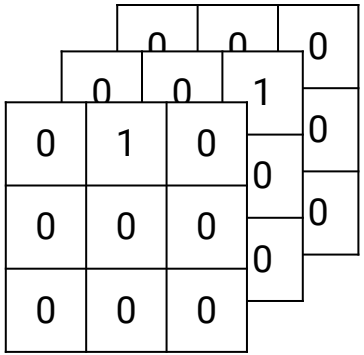
[1] Schlichtkrull et al. Modeling Relational Data with Graph Convolutional Networks. ESWC 2018
[2] William Hamilton. Graph Representation Learning. Morgan & Claypool, 2020
[3] Thanapalasingam et al. Relational Graph Convolutional Networks: A Closer Look. arxiv:2021

Relational GCN (R-GCN) Decoders



[1] Schlichtkrull et al. Modeling Relational Data with Graph Convolutional Networks. ESWC 2018
[2] William Hamilton. Graph Representation Learning. Morgan & Claypool, 2020
[3] Thanapalasingam et al. Relational Graph Convolutional Networks: A Closer Look. arxiv:2021

Relational GCN (R-GCN) Input Formats

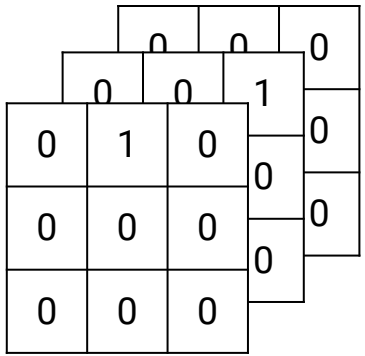


$$\mathcal{T} : \mathbb{R}^{|E| \times |E| \times |R|}$$

- |R| квадратных матриц смежности
- Эффективно только с использованием разреженных матриц (sparse matrices) (scipy.sparse, torch.sparse, etc)

[1] Schlichtkrull et al. Modeling Relational Data with Graph Convolutional Networks. ESWC 2018

Relational GCN (R-GCN) Input Formats



$$\mathcal{T} : \mathbb{R}^{|E| \times |E| \times |R|}$$

- |R| квадратных матриц смежности
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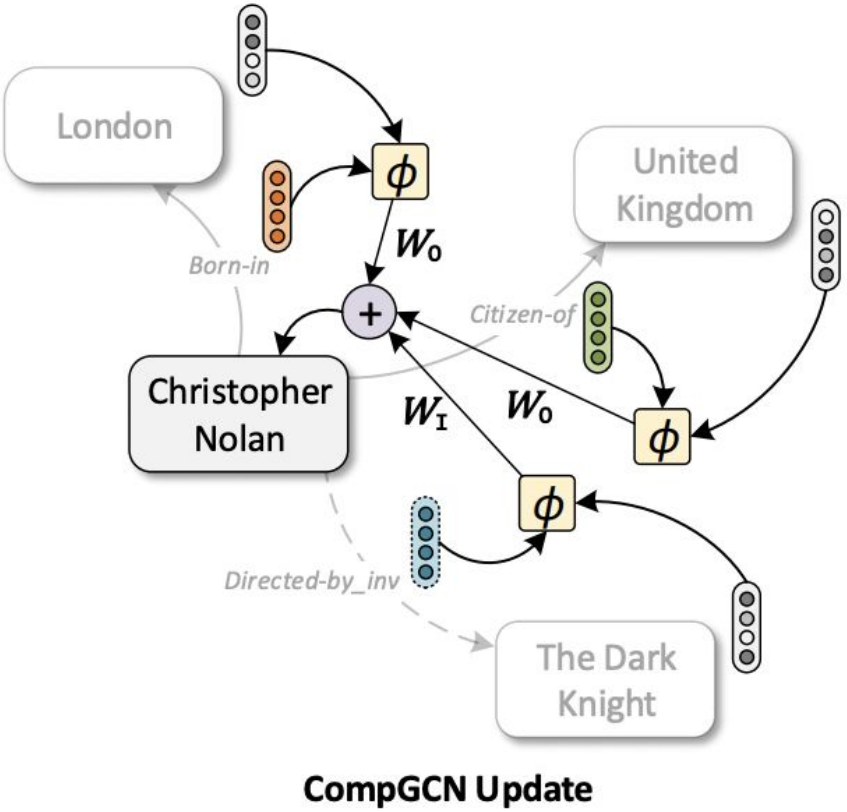
```
r1: [[1, 3, 3, 2, ...], # <- source
     [2, 2, 1, 4, ...]] # <- target

r2: [2, num_edges_r2]
r3: [2, num_edges_r3]
...
r_n: [2, num_edges_rn]
```

- |R| матриц в COO формате (edge index)

[1] Schlichtkrull et al. Modeling Relational Data with Graph Convolutional Networks. ESWC 2018

Compositional GCN (CompGCN)



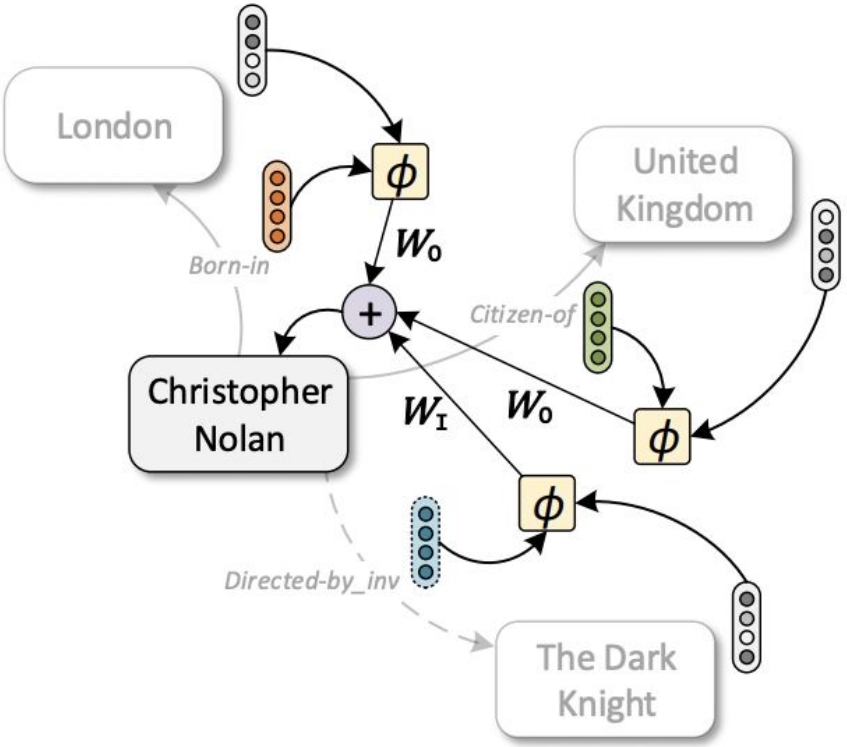
CompGCN Update

$$h_v = f\left(\sum_{(u,r)\in\mathcal{N}(v)} W_{\lambda(r)}\phi(x_u, z_r)\right)$$

- Каждый тип связи параметризуется **вектором z_r**
  - Значительное уменьшение количества параметров
- Сообщения строятся как **композиция** вектора узла и типа связи (функция ϕ)
  - Любая (e,r) функция
  - TransE
  - RotatE, etc

Vashishth et al. Composition-Based Multi-Relational Graph Convolutional Networks. ICLR 2020

Compositional GCN (CompGCN)



CompGCN Update

$$h_v = f\left(\sum_{(u,r)\in\mathcal{N}(v)} W_{\lambda(r)}\phi(x_u, z_r)\right)$$

- Только 3 весовые матрицы **Wλ**
  - Оригинальные связи (direct)
  - Инверсные связи (inverse)
  - Self-loops

$$W_{\text{dir}(r)} = \begin{cases} W_O, & r \in \mathcal{R} \\ W_I, & r \in \mathcal{R}_{inv} \\ W_S, & r = \top \textit{ (self-loop)} \end{cases}$$

Типы связей на следующем слое:

$$h_r = W_{\text{rel}} z_r$$

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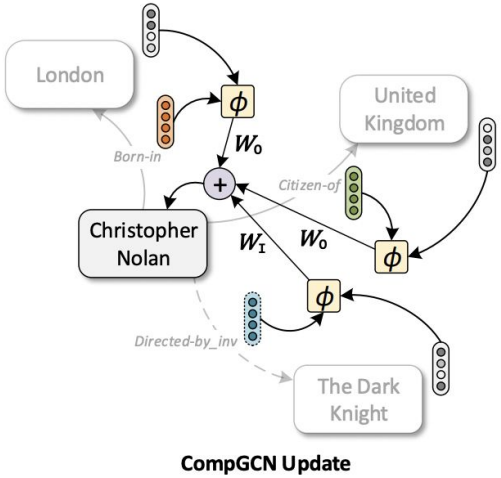
Compositional GCN (CompGCN): COO Input




```
[[1, 3, 3, 2, ...], # <- source
 [2, 2, 1, 4, ...], # <- target
 [0, 1, 1, 2, ...]] # <- edge types
```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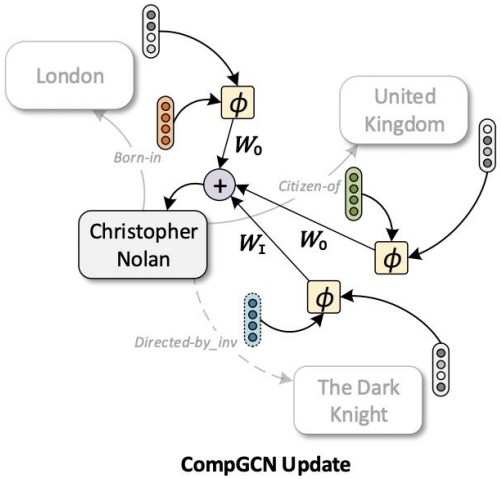
Compositional GCN (CompGCN): COO Input




```
[[1, 3, 3, 2, ...], # <- source
 [2, 2, 1, 4, ...], # <- target
 [0, 1, 1, 2, ...]] # <- edge types
```

```
[[1, 3, 3, 2, ..., 2, 2, 1, 4, ..., 1, 2, 3, 4, ...  ], # <- source
 [2, 2, 1, 4, ..., 1, 3, 3, 2, ..., 1, 2, 3, 4, ...  ], # <- target
 [0, 1, 1, 2, ..., k+1, k+3, k+3, k+2, ..., sl, sl, sl, sl, ... ]] # <- edge types
```

Direct edges

Inverse edges, **new edge types**

Self-loops + special edge type

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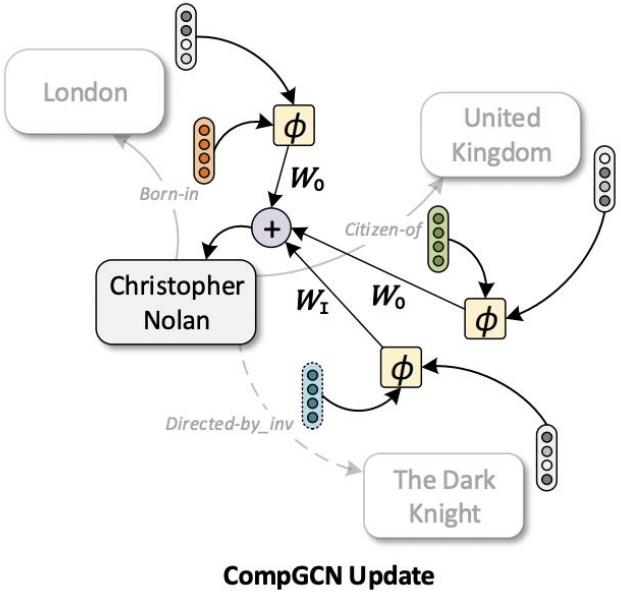
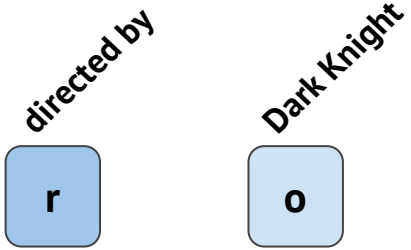
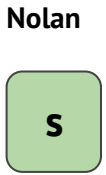
Compositional GCN (CompGCN): COO Input



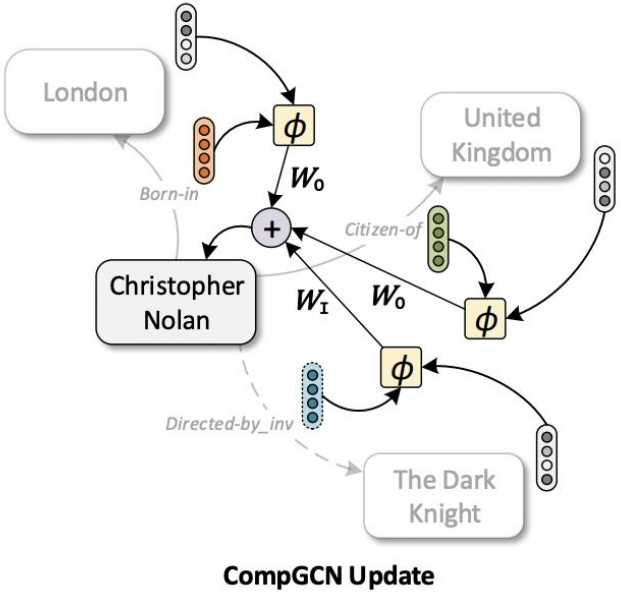
CompGCN Update



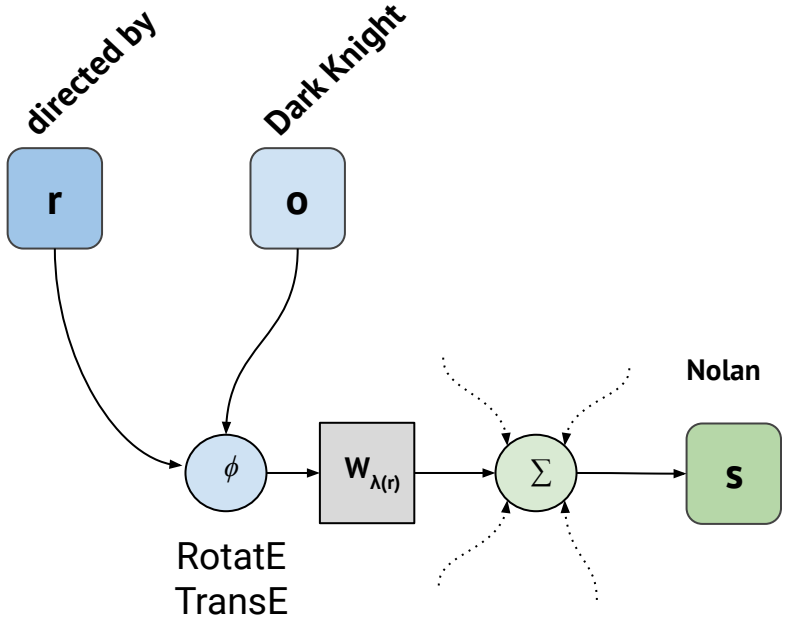


Vashishth et al. Composition-Based Multi-Relational Graph Convolutional Networks. ICLR 2020

Compositional GCN (CompGCN): COO Input



CompGCN Update



RotatE
TransE
DistMult
etc

Vashishth et al. Composition-Based Multi-Relational Graph Convolutional Networks. ICLR 2020

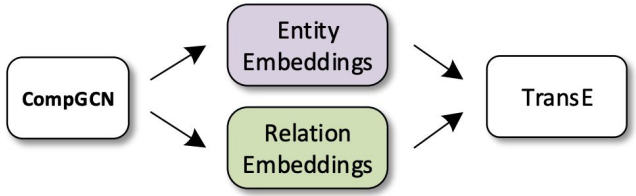
Compositional GCN (CompGCN) - Performance

	FB15k-237					WN18RR				
	MRR	MR	H@10	H@3	H@1	MRR	MR	H@10	H@3	H@1
TransE (Bordes et al., 2013)	.294	357	.465	-	-	.226	3384	.501	-	-
DistMult (Yang et al., 2014)	.241	254	.419	.263	.155	.43	5110	.49	.44	.39
ComplEx (Trouillon et al., 2016)	.247	339	.428	.275	.158	.44	5261	.51	.46	.41
R-GCN (Schlichtkrull et al., 2017)	.248	-	.417		.151	-	-	-		-
KBGAN (Cai & Wang, 2018)	.278	-	.458		-	.214	-	.472	-	-
ConvE (Dettmers et al., 2018)	.325	244	.501	.356	.237	.43	4187	.52	.44	.40
ConvKB (Nguyen et al., 2018)	.243	311	.421	.371	.155	.249	**3324**	.524	.417	.057
SACN (Shang et al., 2019)	.35	-	**.54**	**.39**	.26	.47	-	.54	.48	.43
HypER (Balažević et al., 2019)	.341	250	.520	.376	.252	.465	5798	.522	.477	.436
RotatE (Sun et al., 2019)	.338	**177**	.533	.375	.241	.476	3340	**.571**	.492	.428
ConvR (Jiang et al., 2019)	.350	-	.528	.385	.261	.475	-	.537	.489	**.443**
VR-GCN (Ye et al., 2019)	.248	-	.432	.272	.159	-	-	-	-	-
CompGCN (Proposed Method)	**.355**	197	**.535**	**.390**	**.264**	**.479**	3533	.546	**.494**	**.443**

Vashishth et al. Composition-Based Multi-Relational Graph Convolutional Networks. ICLR 2020

Compositional GCN (CompGCN) - Performance

Как декодер можно взять любую scoring function из shallow моделей (Lecture 7)



Scoring Function (=X) →	TransE			DistMult			ConvE		
Methods ↓	MRR	MR	H@10	MRR	MR	H@10	MRR	MR	H@10
X	0.294	357	0.465	0.241	354	0.419	0.325	244	0.501
X + D-GCN	0.299	351	0.469	0.321	225	0.497	0.344	200	0.524
X + R-GCN	0.281	325	0.443	0.324	230	0.499	0.342	197	0.524
X + W-GCN	0.267	1520	0.444	0.324	229	0.504	0.344	201	0.525
X + CompGCN (Sub)	0.335	**194**	0.514	0.336	231	0.513	0.352	199	0.530
X + CompGCN (Mult)	**0.337**	233	0.515	**0.338**	**200**	**0.518**	0.353	216	0.532
X + CompGCN (Corr)	0.336	214	**0.518**	0.335	227	0.514	**0.355**	197	**0.535**
X + CompGCN ($\mathcal{B} = 50$)	0.330	203	0.502	0.333	210	0.512	0.350	**193**	0.530

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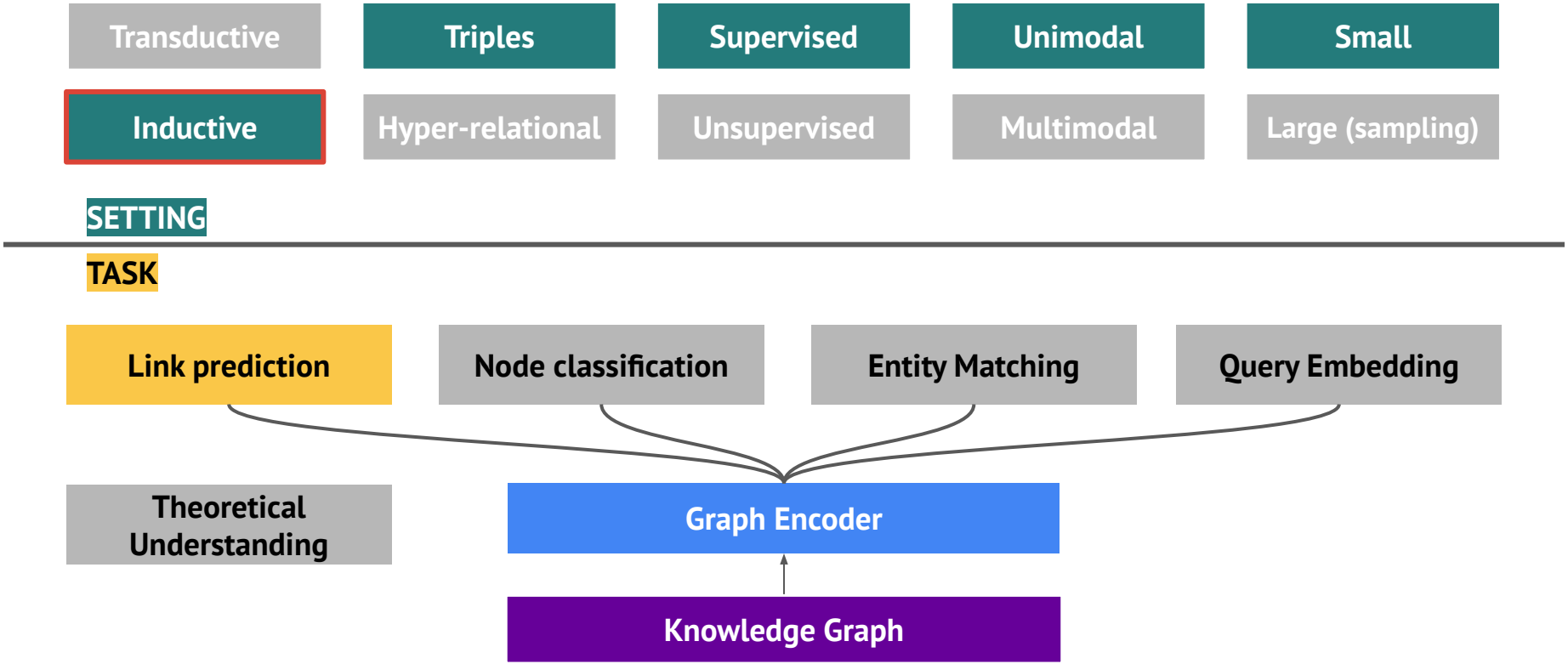
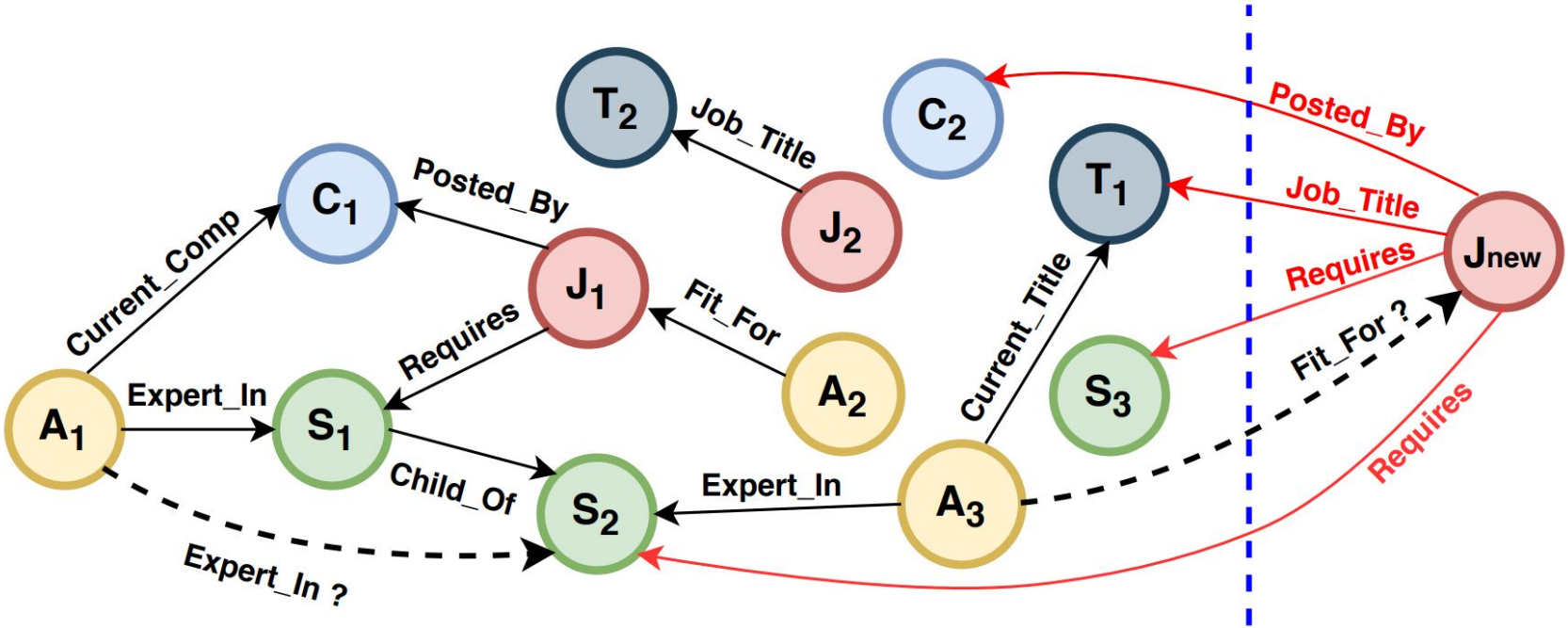
Inductive Learning

Inductive Learning



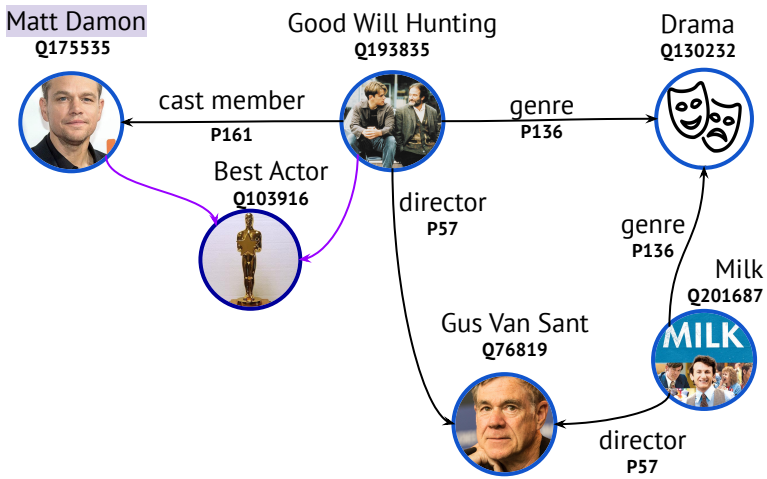
Inductive Learning 1 - Добавление к известному графу



- На инференс приходит новая сущность Jnew, для которой у нас нет эмбеддинга
- Моделирует в т.ч. и темпоральные условия (изменения графа во времени)

Albooyeh et al. Out-of-Sample Representation Learning for Knowledge Graphs. EMNLP 2020

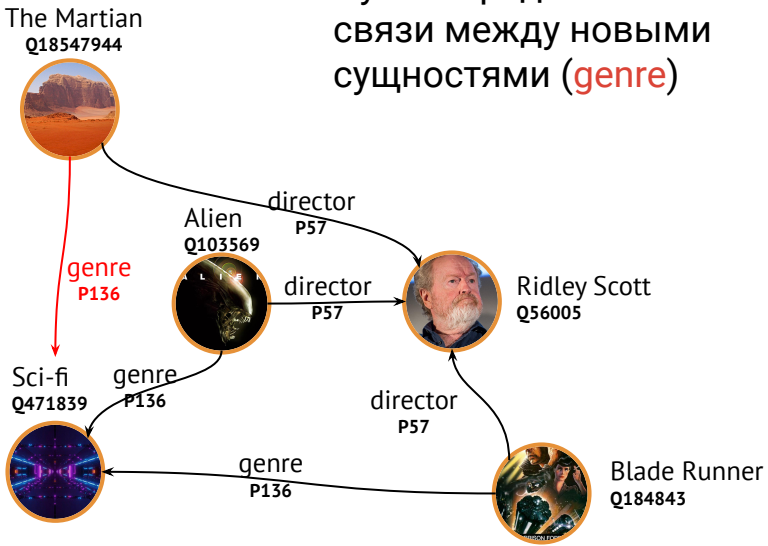
Inductive Learning 2 - Новый инференс граф



Тренировочный граф

Тест (Inference)

- Новые сущности
- Известные предикаты
- Нужно предсказывать связи между новыми сущностями (genre)



Transductive vs Inductive

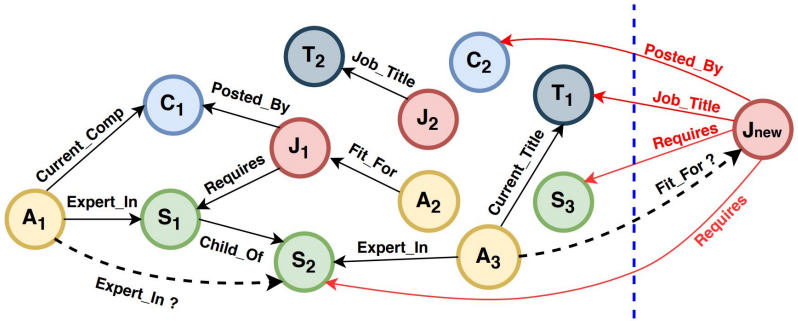
Transductive
(трансдуктивный)

1. Весь граф известен во время тренировки
2. Применимы shallow / decoder-only модели (TransE, RotatE, ConvE, ComplEx, etc) для тренировки
3. Полученная матрица entity embeddings применима на тесте/инференсе

Inductive
(индуктивный)

1. Валидация/тест/инференс - новые сущности или новый граф
   a. Relation types не изменяются
2. Shallow / decoder-only модели не могут выучить эмбеддинг неизвестного узла (unseen node)
   a. **Как построить node feature?**
3. GNNs могут работать в индуктивном сценарии
   a. Используя дополнительные node features
   b. Используя представления подграфов или путей

Inductive Learning 1 - Добавление к известному графу



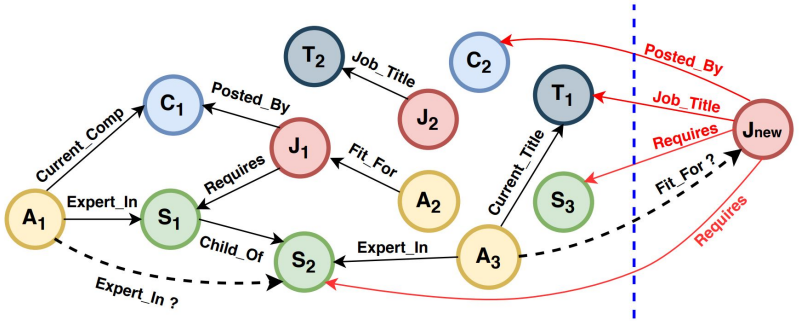
DistMult

$$z_v = \frac{1}{|\mathcal{G}_v|}\left(\sum_{(v,r,u)\in\mathcal{G}_v} z_r \odot z_u + \sum_{(u,r,v)\in\mathcal{G}_v} z_r \odot z_u \right)$$

- Идея: эмбеддинг новой сущности как среднее от представлений соседей

Albooyeh et al. Out-of-Sample Representation Learning for Knowledge Graphs. EMNLP 2020

Inductive Learning 1 - Добавление к известному графу



DistMult

$$\boldsymbol{z}_{\mathsf{v}} = \frac{1}{|\mathcal{G}_{\mathsf{v}}|}\Big(\sum_{(\mathsf{v},\mathsf{r},\mathsf{u})\in\mathcal{G}_{\mathsf{v}}} \boldsymbol{z}_{\mathsf{r}} \odot \boldsymbol{z}_{\mathsf{u}} + \sum_{(\mathsf{u},\mathsf{r},\mathsf{v})\in\mathcal{G}_{\mathsf{v}}} \boldsymbol{z}_{\mathsf{r}} \odot \boldsymbol{z}_{\mathsf{u}} \Big)$$

- Идея: эмбеддинг новой сущности как среднее от представлений соседей
- Новый способ тренировки для имитации “новых” сущностей

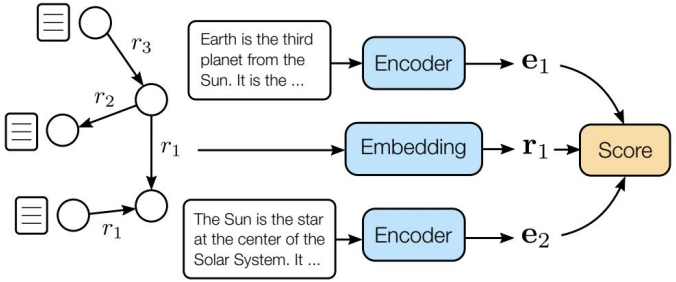
Algorithm 2 Out-of-Sample Training (one epoch)

Inputs n : negative ratio, $\mathcal{L}$: loss function, ψ : see Section 3.1

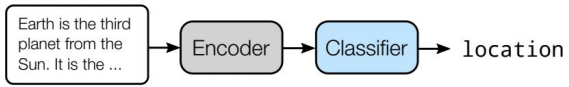
for $batch = 1$ **to** $numBatches$ **do**
  $triples, labels \leftarrow$ `nextBatch` $(batch, n)$
  $scores \leftarrow []$
  for $(\mathsf{v}, \mathsf{r}, \mathsf{u})$ **in** $triples$ **do**
    $\boldsymbol{z}_{\mathsf{r}} \leftarrow \texttt{lookup}(\mathsf{r}, \boldsymbol{Z}_{\mathsf{r}})$
    $rand \leftarrow \texttt{random}()$
    if $rand < \frac{\psi}{2}$ **then**
      $\boldsymbol{z}_{\mathsf{v}} \leftarrow \texttt{aggregate}(\mathsf{v}, \boldsymbol{Z}_{rels}, \boldsymbol{Z}_{ent})$
      $\boldsymbol{z}_{\mathsf{u}} \leftarrow \texttt{lookup}(\mathsf{u}, \boldsymbol{Z}_{ent})$
    else if $\frac{\psi}{2} < rand < \psi$ **then**
      $\boldsymbol{z}_{\mathsf{v}} \leftarrow \texttt{lookup}(\mathsf{v}, \boldsymbol{Z}_{ent})$
      $\boldsymbol{z}_{\mathsf{u}} \leftarrow \texttt{aggregate}(\mathsf{u}, \boldsymbol{Z}_{rel}, \boldsymbol{Z}_{ent})$
    else
      $\boldsymbol{z}_{\mathsf{v}} \leftarrow \texttt{lookup}(\mathsf{v}, \boldsymbol{Z}_{ent})$
      $\boldsymbol{z}_{\mathsf{u}} \leftarrow \texttt{lookup}(\mathsf{u}, \boldsymbol{Z}_{ent})$
    end if
    $scores.\texttt{append}(\phi(\boldsymbol{z}_{\mathsf{v}}, \boldsymbol{z}_{\mathsf{r}}, \boldsymbol{z}_{\mathsf{u}}))$
  end for
  `updateParams`$(\mathcal{L}, scores, labels)$
end for

Albooyeh et al. Out-of-Sample Representation Learning for Knowledge Graphs. EMNLP 2020

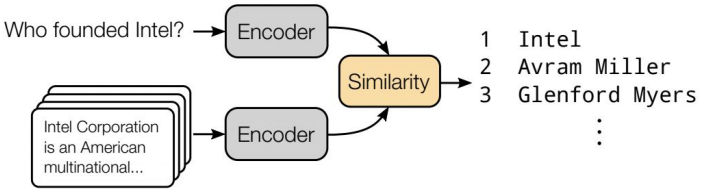
Inductive Learning 2 - Text Descriptions as Features



Link prediction



Entity classification



Information retrieval

- Тренировать эмбеддинги на train graph бессмысленно, **НО** у всех сущностей часто есть текстовое описание (Wikidata, DBpedia, Wikipedia)
- Будем использовать языковую модель (BERT, etc) как универсальный энкодер (featurizer) этих описаний
- Полученные эмбеддинги можно использовать в link prediction, entity classification, IR

Daza et al. Inductive Entity Representations from Text via Link Prediction. WWW 2021

Inductive Learning 2 - Text Descriptions as Features

Стандартная схема: encoder + decoder (task-specific)

- Например, BERT + TransE

	WN18RR				FB15k-237				Wikidata5M			
Method	MRR	H@1	H@3	H@10	MRR	H@1	H@3	H@10	MRR	H@1	H@3	H@10
GloVe-BOW	0.170	0.055	0.215	0.405	0.172	0.099	0.188	0.316	0.343	0.092	0.531	0.756
BE-BOW	0.180	0.045	0.244	0.450	0.173	0.103	0.184	0.316	0.362	0.082	0.586	0.798
GloVe-DKRL	0.115	0.031	0.141	0.282	0.112	0.062	0.111	0.211	0.282	0.077	0.403	0.660
BE-DKRL	0.139	0.048	0.169	0.320	0.144	0.084	0.151	0.263	0.322	0.097	0.474	0.720
KEPLER	–	–	–	–	–	–	–	–	0.402	0.222	0.514	0.730
BLP-TransE	**0.285**	0.135	**0.361**	**0.580**	**0.195**	**0.113**	**0.213**	**0.363**	0.478	0.241	0.660	0.871
BLP-DistMult	0.248	0.135	0.288	0.481	0.146	0.076	0.156	0.286	0.472	0.242	0.646	0.869
BLP-ComplEx	0.261	**0.156**	0.297	0.472	0.148	0.081	0.154	0.283	0.489	0.262	**0.664**	**0.877**
BLP-SimplE	0.239	0.144	0.265	0.435	0.144	0.077	0.152	0.274	**0.493**	**0.289**	0.639	0.866

Daza et al. Inductive Entity Representations from Text via Link Prediction. WWW 2021

Inductive Learning 2 - Subgraphs

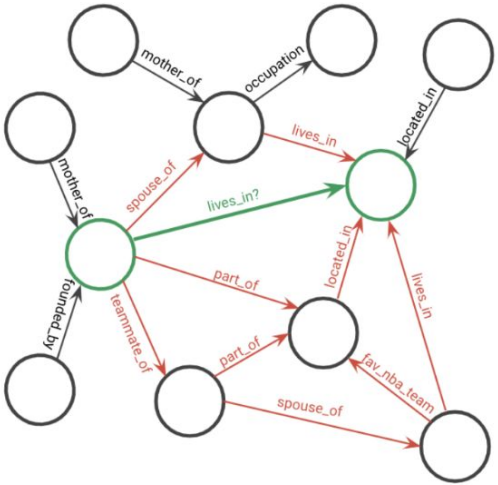
- Текстовых описаний нет
- Откуда брать node embeddings?

Teru et al. Inductive Relation Prediction by Subgraph Reasoning. ICML 2020

Inductive Learning 2 - Subgraphs

- Текстовых описаний нет
- Откуда брать node embeddings?

- Тренируем relation embeddings
- Получаем node features из структуры подграфов (sample subgraphs)



1. Sample the enclosing sub-graph around the link to be predicted (target link).

Сэмплируем подграф вокруг двух заданных узлов

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Inductive Learning 2 - Subgraphs

- Текстовых описаний нет
- Откуда брать node embeddings?

- Тренируем relation embeddings
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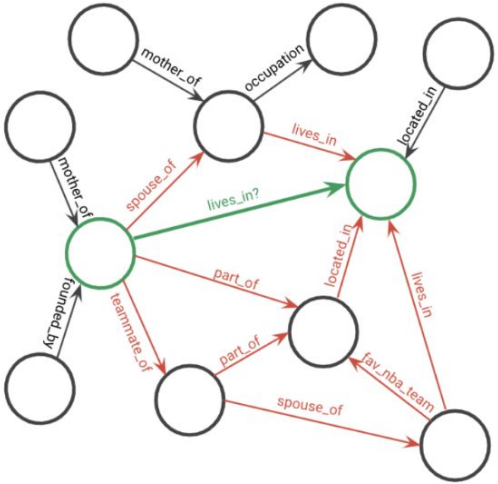

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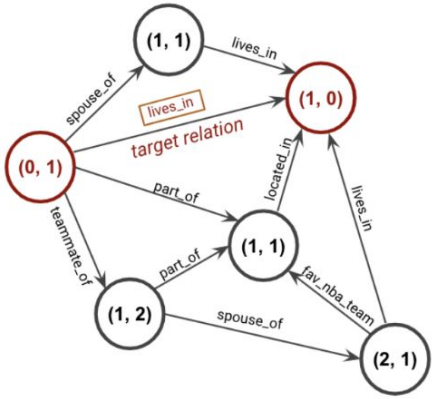

2. Label the nodes w.r.t the target nodes to identify their structural role. Uniquely labels target nodes to mark them for the model.

Получаем кратчайшие пути через алгоритм Дейкстры

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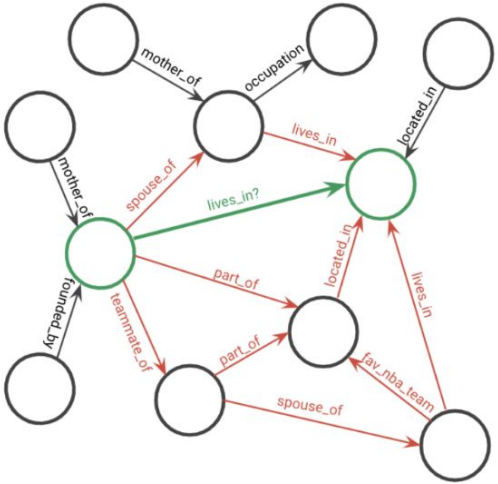

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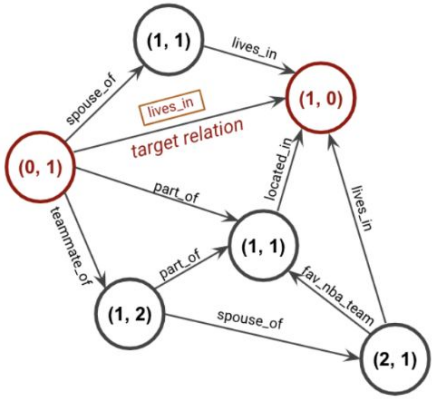

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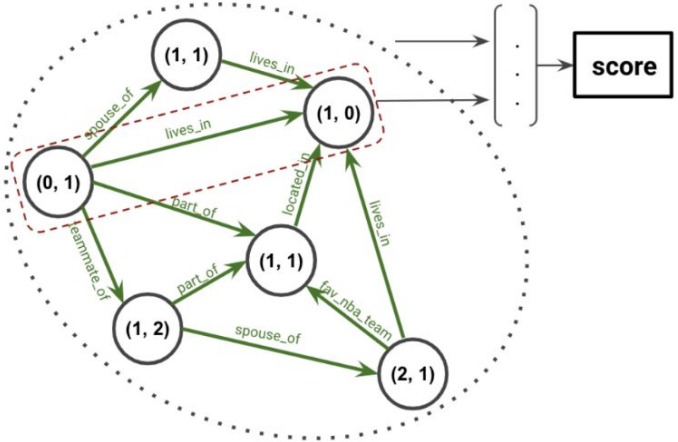

3. Pass messages across the (sub-)graph to predict a score indicating how strongly the structure around the target link supports its logical plausibility.

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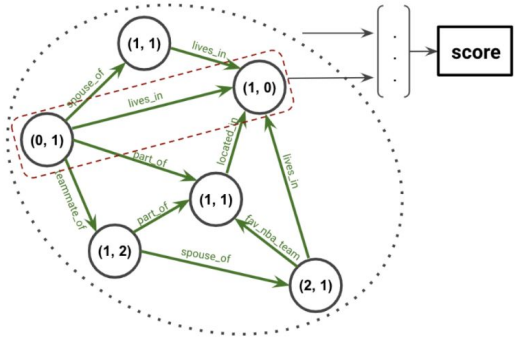
Inductive Learning 2 - Subgraphs - GraIL

1. **Энкодер**: edge-aware R-GCN + attention

Inspired by the multi-relational R-GCN (Schlichtkrull et al., 2017) and edge attention, we define our AGGREGATE function as

$$\mathbf{a}_t^k = \sum_{r=1}^{R} \sum_{s \in \mathcal{N}_r(t)} \alpha_{rr_tst}^k \mathbf{W}_r^k \mathbf{h}_s^{k-1},$$

$$\mathbf{s} = \text{ReLU}\left(\mathbf{A}_1^k [\mathbf{h}_s^{k-1} \oplus \mathbf{h}_t^{k-1} \oplus \mathbf{e}_r^a \oplus \mathbf{e}_{r_t}^a] + \mathbf{b}_1^k\right)$$
$$\alpha_{rr_tst}^k = \sigma\left(\mathbf{A}_2^k \mathbf{s} + \mathbf{b}_2^k\right).$$



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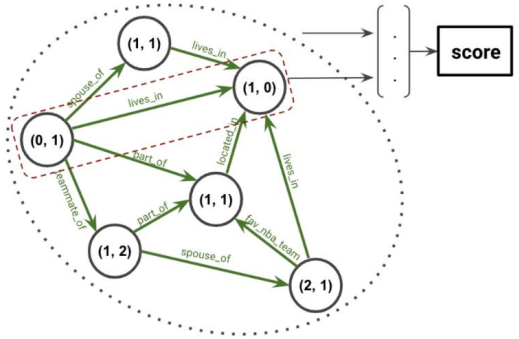
2. **Pooling**: subgraph vector как среднее от представлений его узлов

$$\mathbf{h}_{\mathcal{G}_{(u,v,r_t)}}^L = \frac{1}{|\mathcal{V}|} \sum_{i \in \mathcal{V}} \mathbf{h}_i^L,$$

3. **Финальный декодер**

$$\text{score}(u, r_t, v) = \mathbf{W}^T [\mathbf{h}_{\mathcal{G}_{(u,v,r_t)}}^L \oplus \mathbf{h}_u^L \oplus \mathbf{h}_v^L \oplus \mathbf{e}_{r_t}].$$



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Inductive Learning 2 - Subgraphs - GraIL

Только relation prediction (не link prediction) из-за высокой вычислительной сложности

Table 1. Inductive results (AUC-PR)

	WN18RR				FB15k-237				NELL-995			
	v1	v2	v3	v4	v1	v2	v3	v4	v1	v2	v3	v4
Neural-LP	86.02	83.78	62.90	82.06	69.64	76.55	73.95	75.74	64.66	83.61	87.58	85.69
DRUM	86.02	84.05	63.20	82.06	69.71	76.44	74.03	76.20	59.86	83.99	87.71	85.94
RuleN	90.26	89.01	76.46	85.75	75.24	88.70	91.24	91.79	84.99	88.40	87.20	80.52
GraIL	**94.32**	**94.18**	**85.80**	**92.72**	**84.69**	**90.57**	**91.68**	**94.46**	**86.05**	**92.62**	**93.34**	**87.50**

Table 7. Ablation study of the proposed framework (AUC-PR)

	FB (v3)	NELL (v3)
GraIL	**91.68**	**93.34**
GraIL w/o enclosing subgraph	84.25	85.89
GraIL w/o node labeling scheme	82.07	84.46
GraIL w/o attention in GNN	90.27	87.30

Представления подграфов и способ составления node features очень важны

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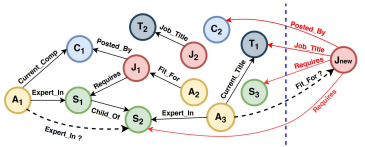
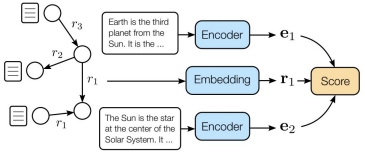
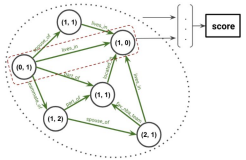
Inductive Learning Summary

Как строим представления неизвестных узлов на инференсе?	Сценарий	Способ
Агрегация тренированных векторов известных нод	Новые узлы (инференс) присоединяются к тренировочному графу (out-of-sample)	
Есть текстовые описания узлов	1. Out-of-sample 2. Полностью новый граф	
Совсем никаких заготовленных features. Только структурные свойства графа	1. Out-of-sample 2. Полностью новый граф	

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В следующей серии

1. Introduction
2. Представление знаний в графах - RDF & RDFS & OWL
3. Хранение знаний в графах - SPARQL & Graph Databases
4. Однородность знаний - RDF* & Wikidata & SHACL & ShEx
5. Интеграция данных в графы знаний - Semantic Data Integration
6. Введение в теорию графов - Graph Theory Intro
7. Векторные представления графов - Knowledge Graph Embeddings
8. Машинное обучение на графах - Graph Neural Networks & KGs
9. **Некоторые применения - Question Answering & Query Embedding**