

# Введение в GNN

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# План лекции

**01.** Обзор кейсов ”в ширину”

**02.** Перспективные направления исследований

**03.** Современный стек в графах

**04.** Базовые понятия и приемы в GNN

**05.** Где брать актуальную информацию: полезные ресурсы, курсы и персоналии

# План семинара

**01.** Детальный пайплайн подготовки данных для обучения GNN

**02.** GraphSAGE

**03.** Обучение GNN на задаче бинарной классификации

# Дисклеймеры

**01.** Много ссылок и материалов

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**01.** Много ссылок и материалов

**02.** Не все статьи я помню детально



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**04.** Выводы и информация актуальна на начало ноября 2023,  
но мир меняется очень быстро

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**04.** Выводы и информация актуальна на начало ноября 2023,  
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**05.** Впереди много интересного и максимальная отдача на пересечении  
областей знаний – LLM точно не заменит собой весь AI/DS

# Кейсы

# 01

# 1. RecSys



<https://recsys.acm.org/recsys23/session-6/>

Session-based Recommendation with Graph Neural Networks (2018)

<https://arxiv.org/pdf/1811.00855v4.pdf>

The Kaggle logo, consisting of the word "kaggle" in a blue, lowercase, sans-serif font, enclosed within a light blue rounded rectangular border.

## **2023 OTTO – Multi-Objective Recommender System**

Build a recommender system based on real-world e-commerce sessions  
(30 000\$ prize, 2 574 teams)

<https://www.kaggle.com/competitions/otto-recommender-system>

## **7-е место**

<https://www.kaggle.com/competitions/otto-recommendersystem/discussion/383769>

# 1. RecSys

kaggle

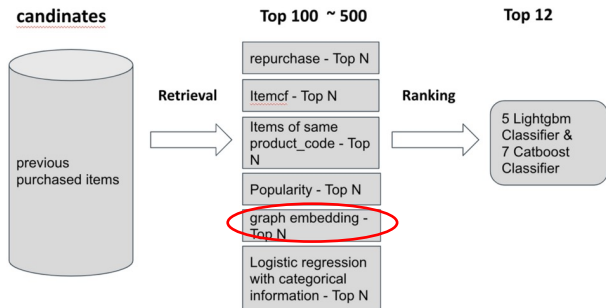
## 2022 H&M Personalized Fashion Recommendations

Provide product recommendations based on previous purchases  
(50 000\$ prize, 2 952 teams)

<https://www.kaggle.com/competitions/h-and-m-personalized-fashion-recommendations>

### 1-е место

<https://www.kaggle.com/competitions/h-and-m-personalized-fashion-recommendations/discussion/324070>



One question is what's the improvement of graph embedding in your recalling and ranking? That's a part which I wanna try but didn't have enough time.

Thanks for your sharing.

← Reply



**senkin13** Posted a year ago · 1st in this Competition TOPIC AUTHOR

about 0.002 up

← Reply



**sirius** Posted a year ago · 3rd in this Competition

Wow, that's really powerful!



# 1. RecSys



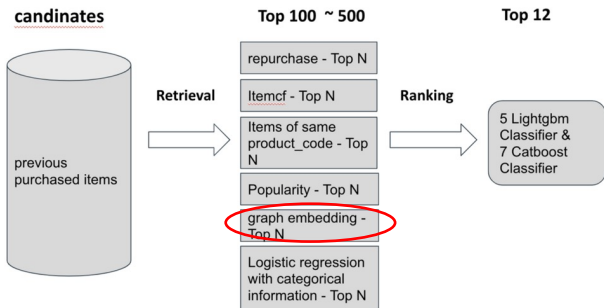
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### 1-е место

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← Reply



**sirius** Posted a year ago · 3rd in this Competition

Wow, that's really powerful!

<https://arxiv.org/abs/2311.00423v1>

LLMRec: Large Language Models with Graph Augmentation for Recommendation. LLMRec - это новый фреймворк и датасет, улучшающий рекомендательные системы путем применения простых, но эффективных стратегий дополнения графов на основе LLM.

– Статья принята на WSDM'24

## 2. Supply chains management

**Цель:** купить дешевле, вовремя  
(когда у других дефицит), снизить  
риски дефицита у себя  
(сможет ли цепь выполнить заказ?)



Кусочек модельной цепи поставок

**Насколько такие цепи прозрачны?**

Контракты конфиденциальны:

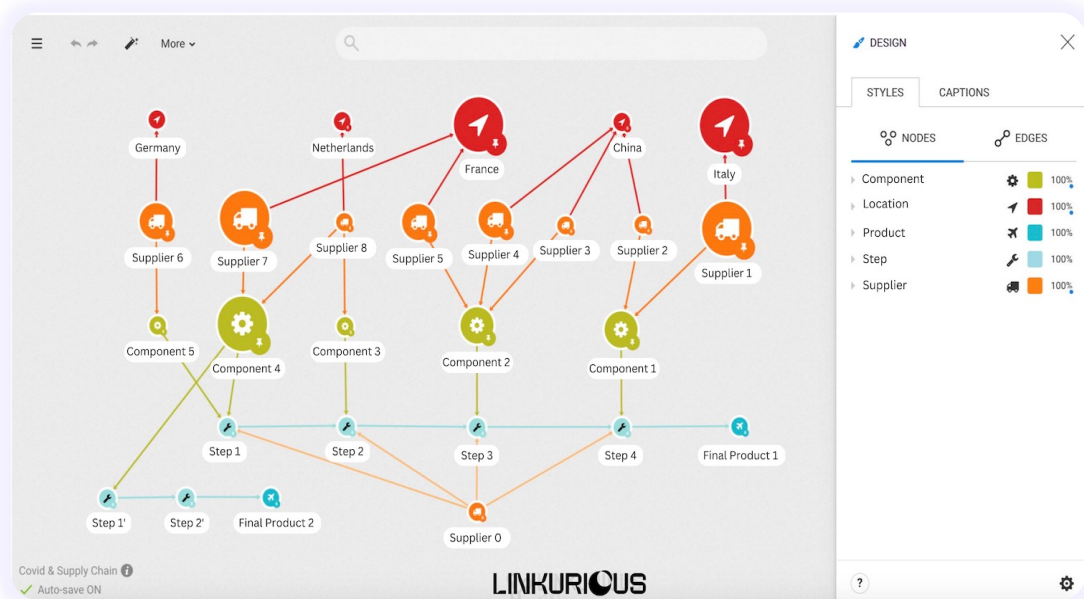
- Кто, кому, сколько, по какой цене?
- А в будущем?

**Кто ключевой связующий поставщик?**  
(Nexus supplier)



Supply Chain Link Prediction on Uncertain Knowledge Graph  
[https://kdd.org/exploration\\_files/p124-AI4Manufacturing\\_paper5.pdf](https://kdd.org/exploration_files/p124-AI4Manufacturing_paper5.pdf)

Чуть далее: извлечение цепочки поставок из новостей  
Extracting supply chain maps from news articles using deep neural networks (2020)  
<https://api.repository.cam.ac.uk/server/api/core/bitstreams/1494b97c-0c4b-4a7b-a562-10e1b0d11586/content>



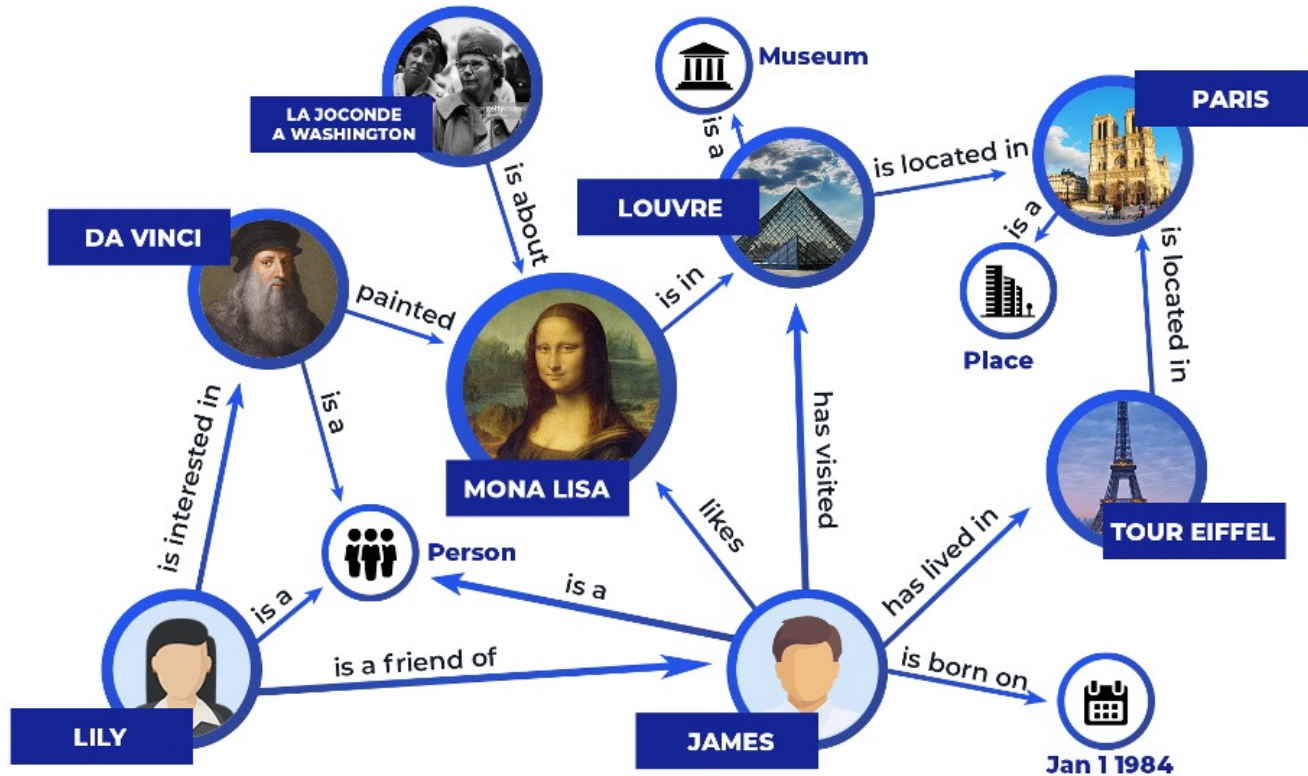
<https://linkurious.com/blog/supply-chain-data-analysis/>



**Cambridge University**

<https://dl.acm.org/doi/abs/10.1145/3575637.3575655>  
<https://api.repository.cam.ac.uk/server/api/core/bitstreams/92a7b226-2f41-4703-ad15-69c53ec7f26a/content>  
<https://github.com/grandintegrator/Link-Prediction-Supply-Chains>

### 3. Knowledge graph

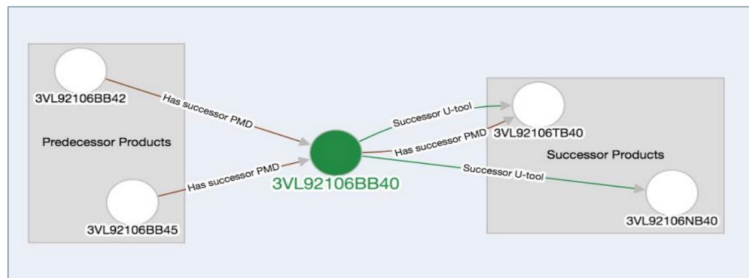
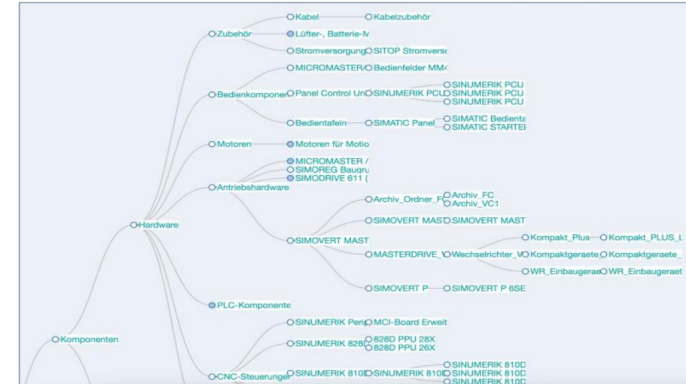
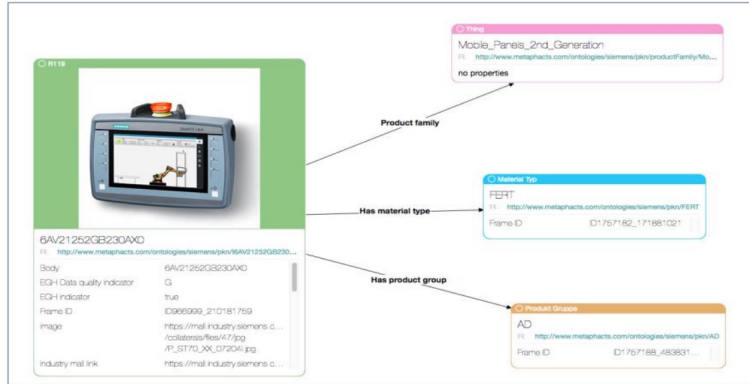


# 3. Knowledge graph (Siemens, 2017)

## Graph Visualization and Exploration

SIEMENS

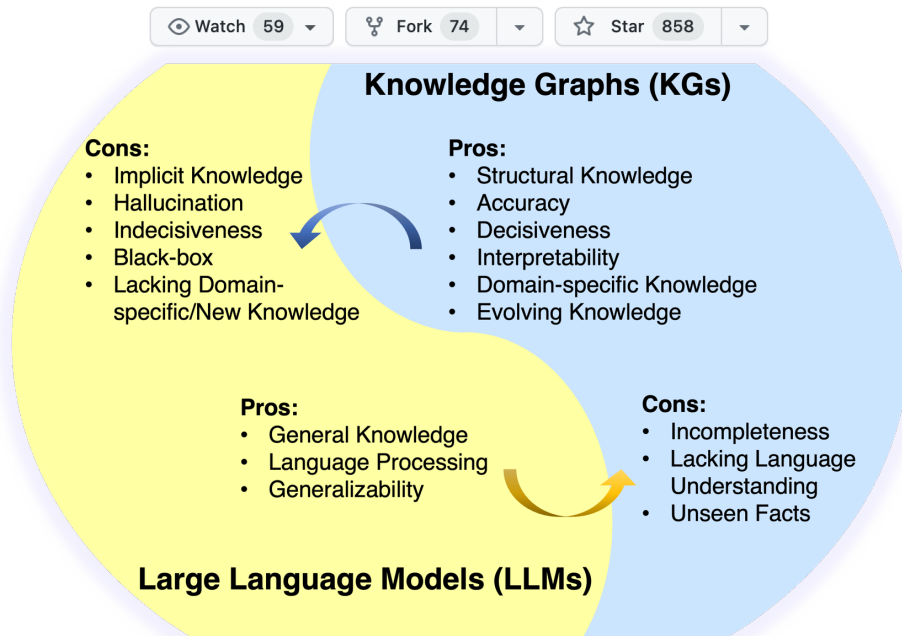
*Ingenuity for life*



### Variety of graph structures:

- Product metadata and relationships
- Successor, predecessor network
- Taxonomic information

### 3. Robust reasoning over Knowledge Graph with LLM (2023)



<https://github.com/RManLuo/Awesome-LLM-KG>

Towards foundation models for knowledge graph reasoning

<https://arxiv.org/pdf/2310.04562.pdf>

<https://towardsdatascience.com/ultra-foundation-models-for-knowledge-graph-reasoning-9f8f4a0d7f09>



NEURAL INFORMATION  
PROCESSING SYSTEMS

Do Temporal Knowledge Graph Embedding Models Learn or Memorize


<https://openreview.net/forum?id=UMokRwWfLW>

**Правила показали около-SOTA результаты, причина – лики при обучении KG-эмбеддингов**



## 4. Document understanding (link prediction)

<https://paperswithcode.com/sota/entity-linking-on-funsd?p=doc2graph-a-task-agnostic-document>










Filter: <span>untagged</span>		● Other models    ➡ Models with highest F1						<span>Edit Leaderboard</span>	
Rank	Model	F1	↑ Paper	Code	Result	Year	Tags		
1	<b>TPP</b> (LayoutMask)	79.23	<a href="#">Reading Order Matters: Information Extraction from Visually-rich Documents by Token Path Prediction</a>		→	2023		<b>13 октября</b>	
2	<b>SINGU_GROUP</b>	70.51	<a href="#">DGCN Based Solution for Entity Linking on Visual Rich Document</a>		→	2022			
3	<b>SERA</b>	65.96	<a href="#">Entity Relation Extraction as Dependency Parsing in Visually Rich Documents</a>		→	2021			
4	<b>Doc2Graph</b>	53.36	<a href="#">Doc2Graph: a Task Agnostic Document Understanding Framework based on Graph Neural Networks</a>		→	2022			

**Doc2Graph: a Task Agnostic Document Understanding Framework based on Graph Neural Networks (2022)**

<https://arxiv.org/abs/2208.11168>

<https://github.com/andreagemelli/doc2graph>

## 5. Fraud detection – GTAN – SOTA на датасетах Amazon-Fraud и Yelp-Fraud

Rank	Model	AUC- ↑ ROC	Averaged Precision	Paper	Code	Result	Year	Tags 🔖
1	GTAN	97.50	89.26	<a href="#">Semi-supervised Credit Card Fraud Detection via Attribute-driven Graph Representation</a>			2023	
2	RLC-GNN	97.48		<a href="#">RLC-GNN: An Improved Deep Architecture for Spatial-Based Graph Neural Network with Application to Fraud Detection</a>			2021	
3	RioGNN	96.19		<a href="#">Reinforced Neighborhood Selection Guided Multi-Relational Graph Neural Networks</a>			2021	
4	PC-GNN	95.86	85.49	<a href="#">Pick and Choose: A GNN-based Imbalanced Learning Approach for Fraud Detection</a>			2021	
5	CARE-GNN	89.73	82.19	<a href="#">Enhancing Graph Neural Network-based Fraud Detectors against Camouflaged Fraudsters</a>			2020	

<https://paperswithcode.com/sota/fraud-detection-on-amazon-fraud>

<https://arxiv.org/pdf/2307.05633.pdf>

<https://arxiv.org/pdf/2205.13084.pdf>

# Кейсы в финансах

## 6. Probability of Default



**Financial Default Prediction via Motif-preserving Graph Neural Network with Curriculum Learning (2023)**

<https://dl.acm.org/doi/abs/10.1145/3580305.3599351>

## 7. AML (anti-money laundering)

**Finding Money Launderers Using Heterogeneous Graph Neural Networks (2023)**

<https://arxiv.org/abs/2307.13499>

## 8. Portfolio management

**Graph Neural Networks for Asset Management (2021)**

<https://research-center.amundi.com/files/nuxeo/dl/52877ebd-db7c-4ddd-95dc-b77f6b5bcf52>

**Multi-Level Graph Neural Network for Information Fusion in Learning Stock Market Dynamics (2023)**

[https://papers.ssrn.com/sol3/papers.cfm?abstract\\_id=4423354](https://papers.ssrn.com/sol3/papers.cfm?abstract_id=4423354)

# 9. ETA (estimated time of arrival) and traffic prediction -- SOTA

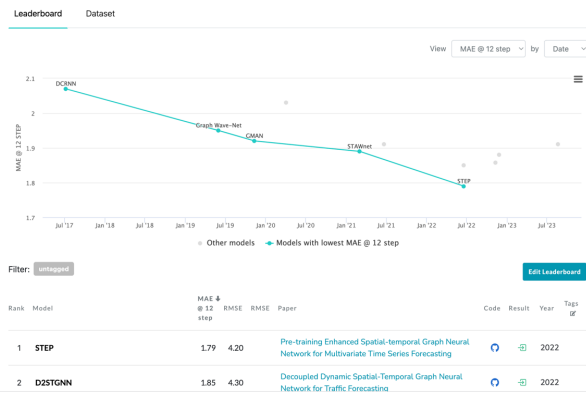


## ETA Prediction with Graph Neural Networks in Google Maps (2021)

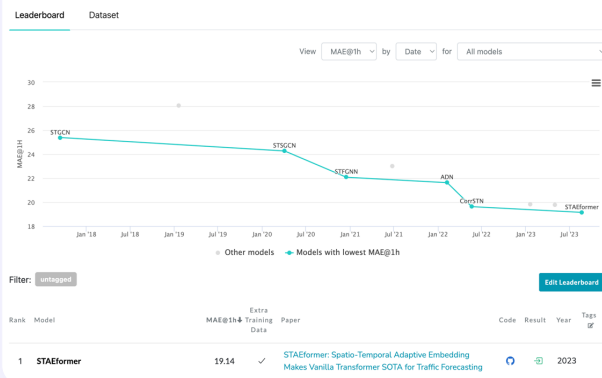
<https://arxiv.org/pdf/2108.11482.pdf>

<https://www.youtube.com/watch?v=zpDdvI95igc>

### Traffic Prediction on PEMS-BAY



### Traffic Prediction on PeMS07



Estimating package arrival time via heterogeneous hypergraph neural network (2023)

<https://www.sciencedirect.com/science/article/abs/pii/S095741742302242X>

Multi-attention graph neural networks for city-wide bus travel time estimation using limited data (2022)

<https://www.sciencedirect.com/science/article/abs/pii/S0957417422004717>

<https://paperswithcode.com/sota/traffic-prediction-on-pems-bay>

<https://paperswithcode.com/sota/traffic-prediction-on-pems07>

# 10. Causal Learning

Relating Graph Neural Networks to Structural Causal Models (2021) (Graph VAE)

<https://arxiv.org/pdf/2109.04173.pdf>

<https://www.youtube.com/watch?v=XC-Bfg3dO0I>



CausalGNN: Causal-Based Graph Neural Networks for Spatio-Temporal Epidemic Forecasting (2022)

<https://ojs.aaai.org/index.php/AAAI/article/view/21479>

Hierarchical Graph Neural Networks for Causal Discovery and Root Cause Localization (2023)

<https://arxiv.org/pdf/2302.01987.pdf>

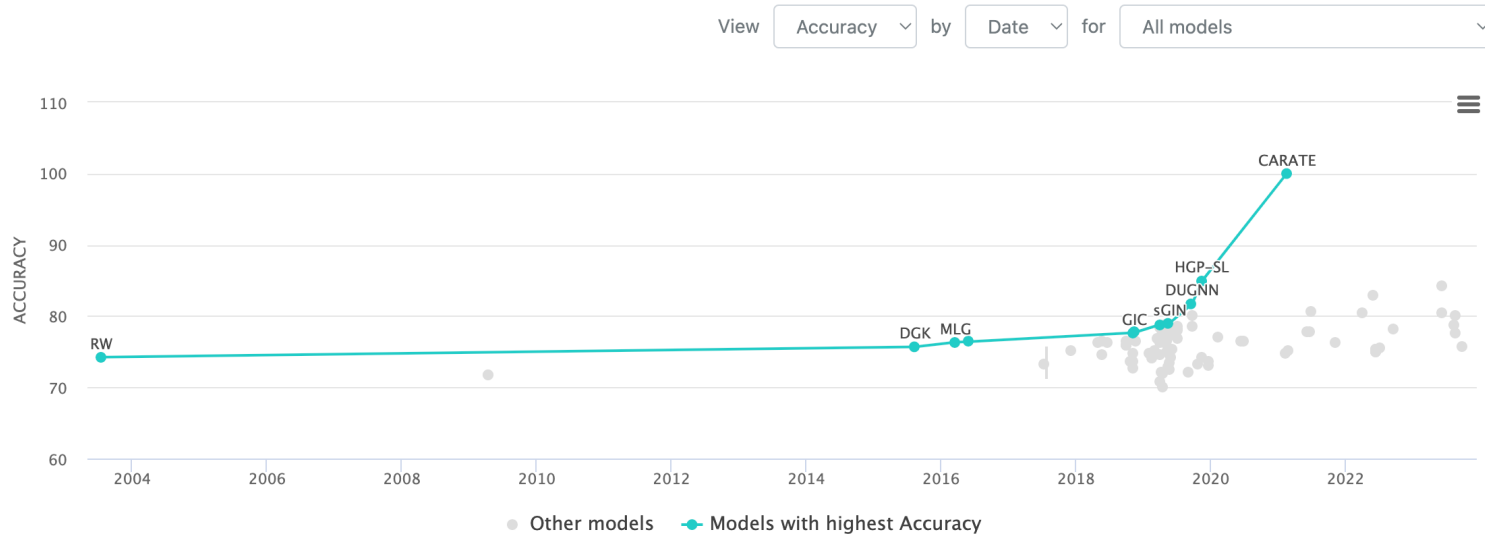
<https://www.youtube.com/watch?v=AStrI3FhMWg>

# 11. Molecular embeddings (88 моделей и все с GNN) – SOTA

## Graph Classification on PROTEINS

Leaderboard

Dataset



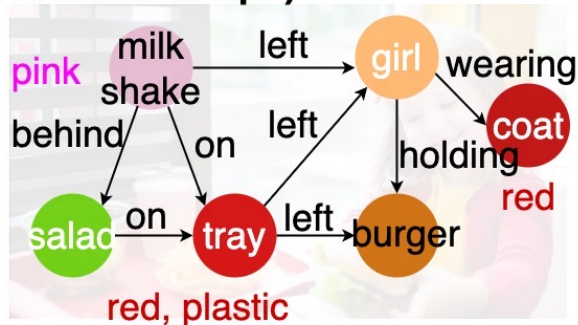
Бинарная классификация – энзим / не энзим

<https://paperswithcode.com/sota/graph-classification-on-proteins>



# 12. Visual query answering (2019 - now)

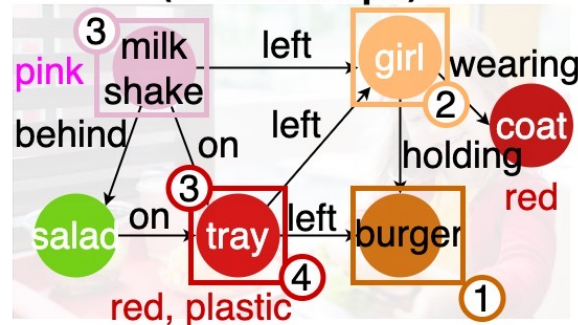
**Input: Image**  
(Represented as A Scene Graph)



**Input: Question**

What is the **red object** left of the **girl** that is holding a **hamburger**?

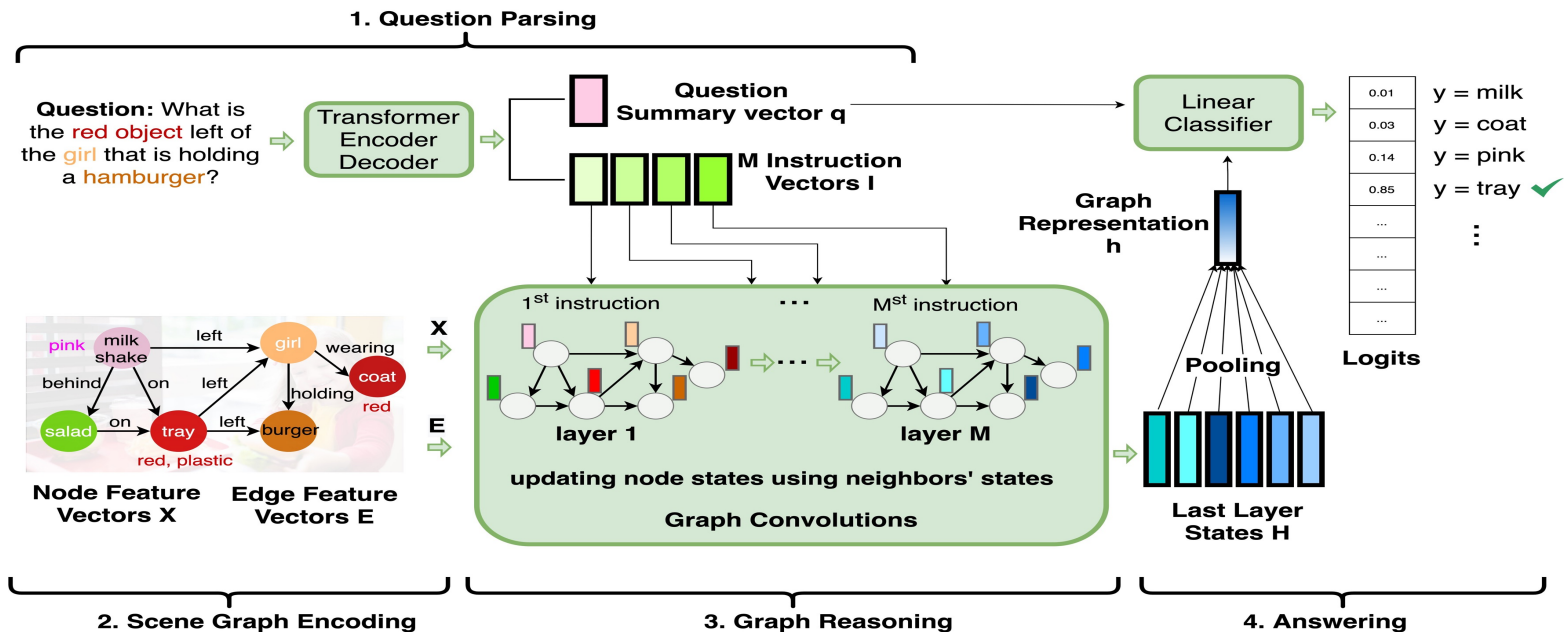
**Step 1: Scene Graph Reasoning**  
(4 Time Steps)



**Step 2: Answer Prediction**

**Answer:** Tray  
(Graph Classification Problem)

# 12. Visual query answering



<https://github.com/codexxxl/GraphVQA>

ICCV23  
PARIS

1st Workshop on Scene Graphs and Graph Representation Learning  
[https://openaccess.thecvf.com/ICCV2023\\_workshops/SG2RL](https://openaccess.thecvf.com/ICCV2023_workshops/SG2RL)

# 13. Прогноз погоды – SOTA

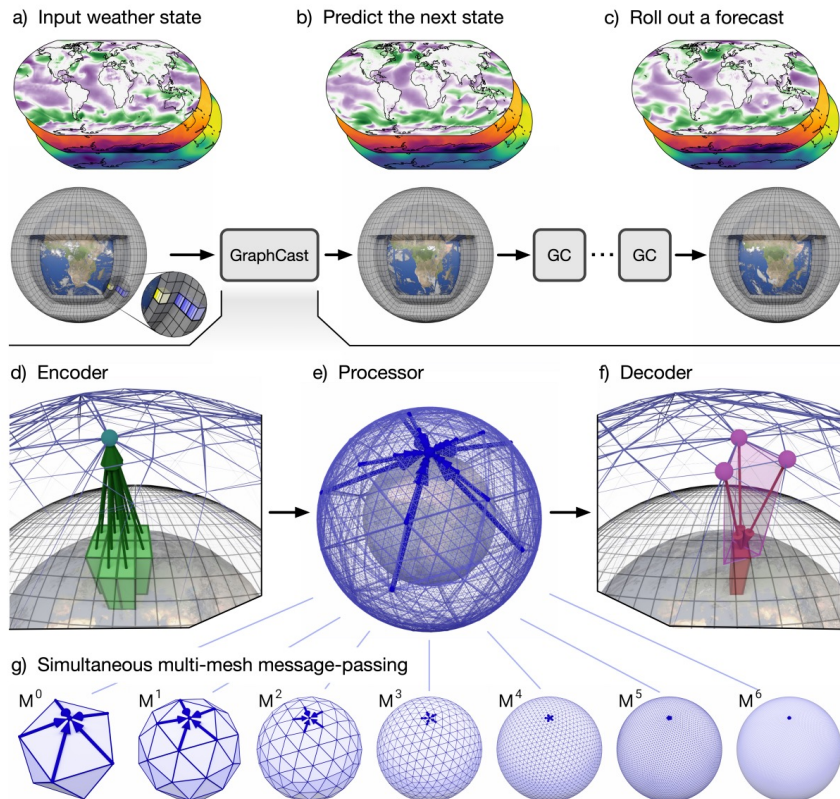


## GraphCast: Learning skillful medium-range global weather forecasting (24.12.2022)

<https://arxiv.org/pdf/2212.12794v2.pdf>

<https://github.com/google-deepmind/graphcast>

<https://paperswithcode.com/paper/graphcast-learning-skillful-medium-range>



## 14. Социальные сети и СМИ – SOTA

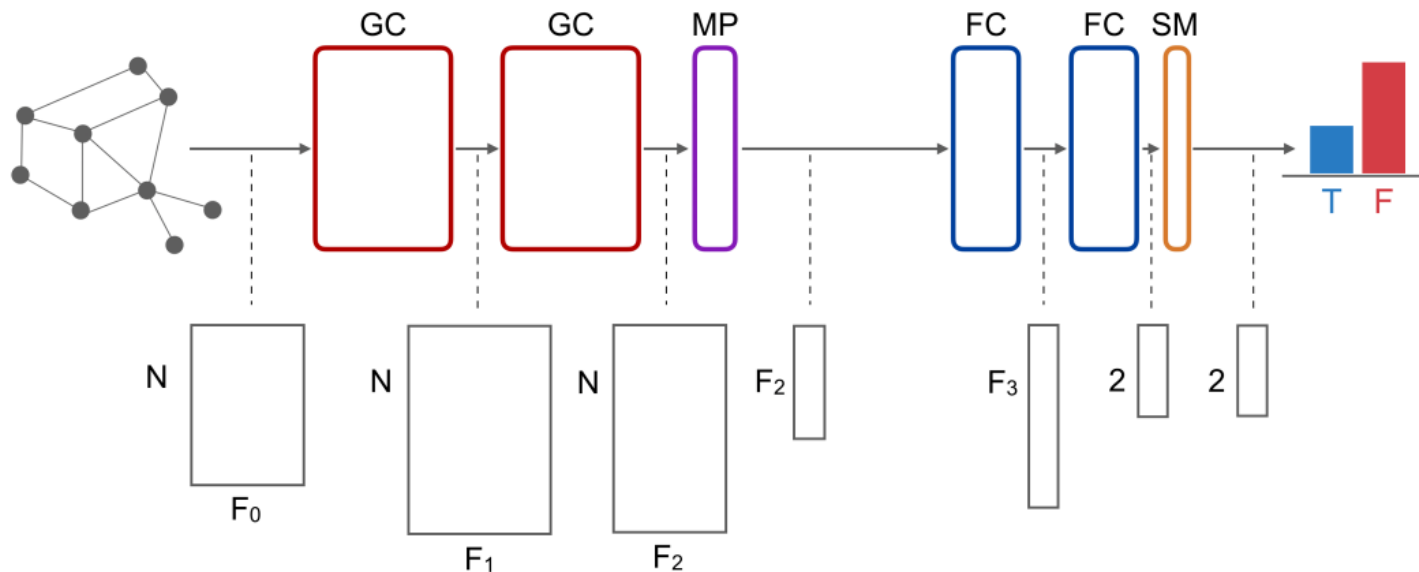
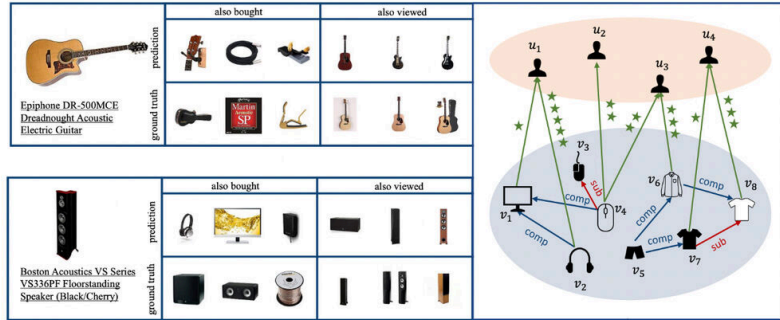


Figure 5: The architecture of our neural network model. Top row: GC = Graph Convolution, MP = Mean Pooling, FC = Fully Connected, SM = SoftMax layer. Bottom row: input/output tensors received/produced by each layer.

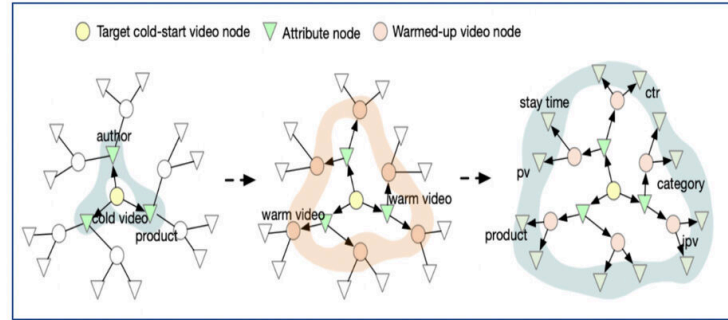
Подборка кейсов (2022) от  
[Nikita Iserson](#)

## Graph Neural Networks for E-Commerce

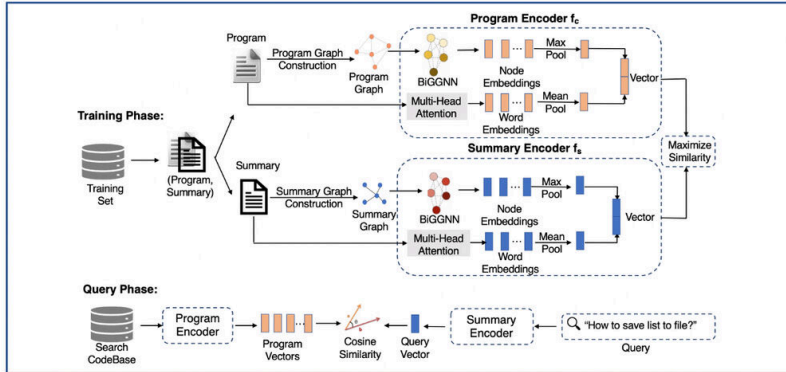
### Product Matching, Item Relationship Prediction



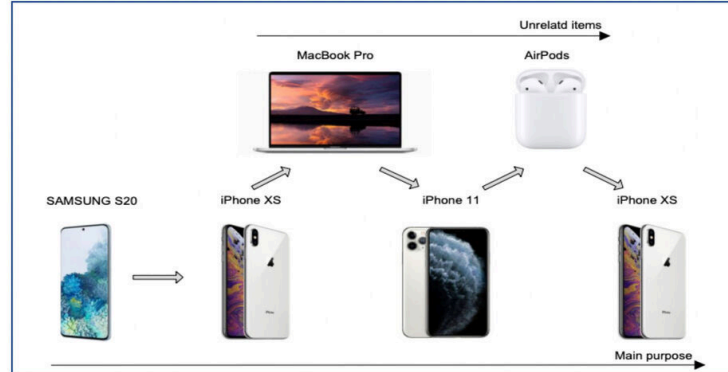
### New Product / New Shop Forecasting / Strict Cold Start



### Improving Search Relevance and Information Retrieval



### Session-Based Recommendation and Click Models

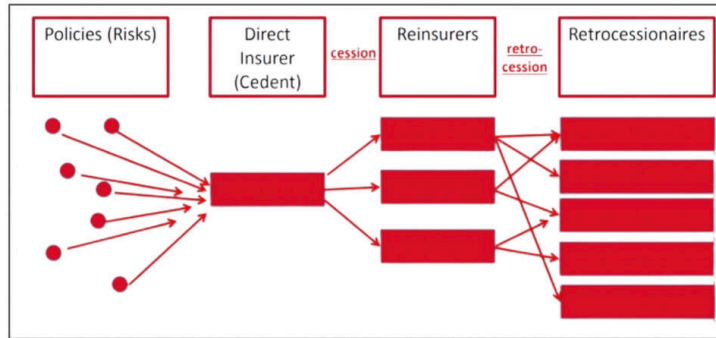




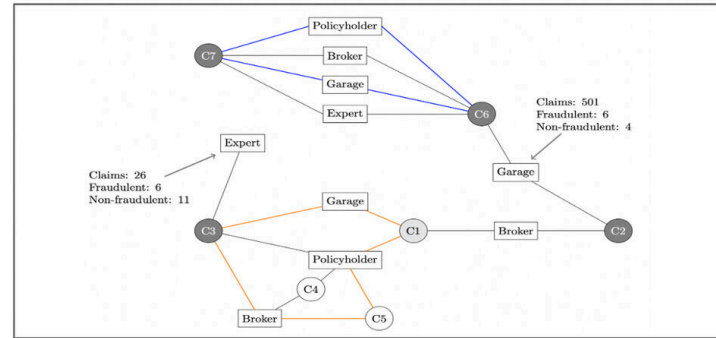
# 2ni. Страхование

## Graph Neural Networks for Insurance

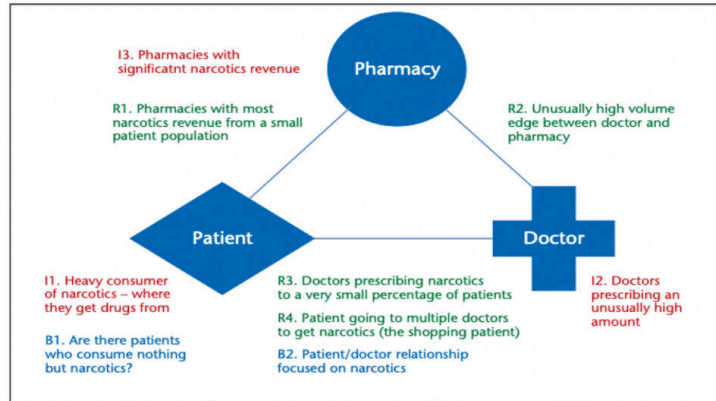
### Modeling Risk, Reinsurance Networks, Cascading Losses



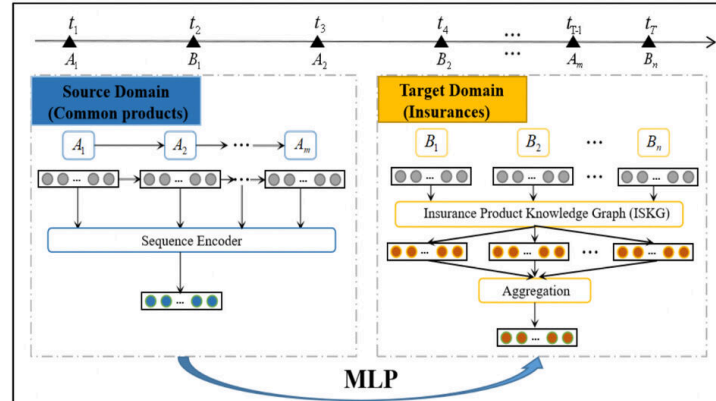
### Fraud Detection in Motor Insurance Sector



### Healthcare & Medicare (Treatment, Actuarial, Fraud & Abuse)



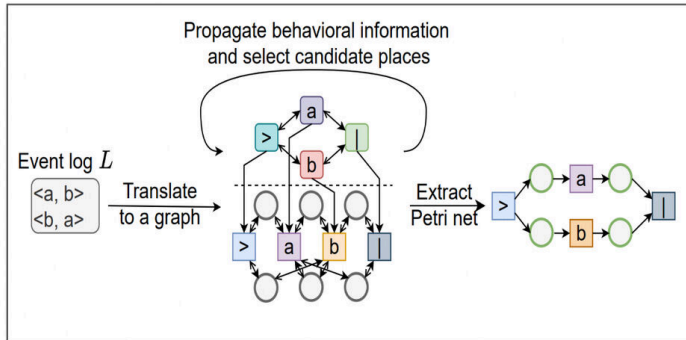
### Recommender Systems and CyberInsurance Ratemaking



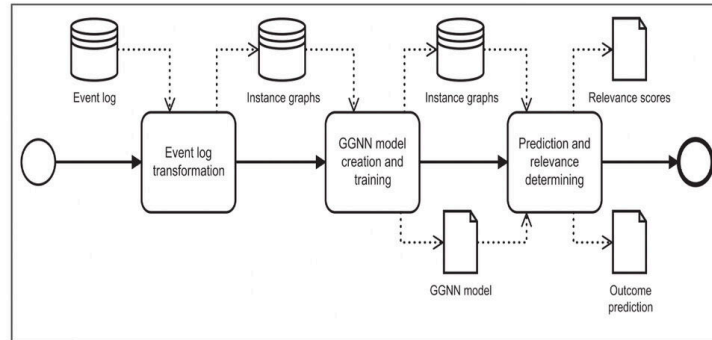
# 3ni. Process Mining

## Graph Neural Networks for Process Analytics

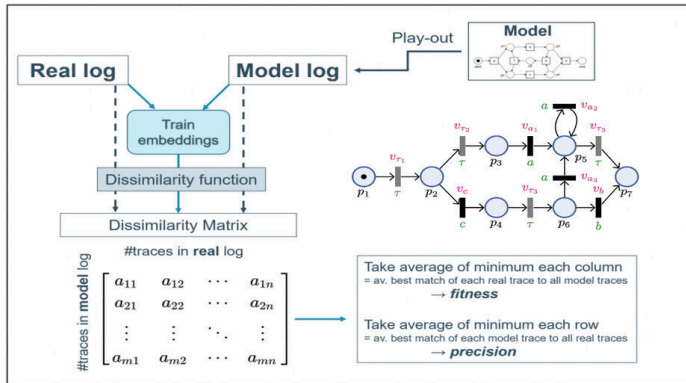
### Process Discovery



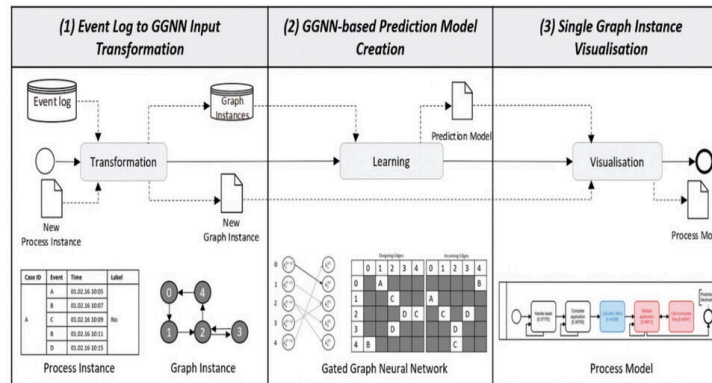
### Process Monitoring (Activity - KPI Relevance)



### Conformance Checking & Trace Embedding

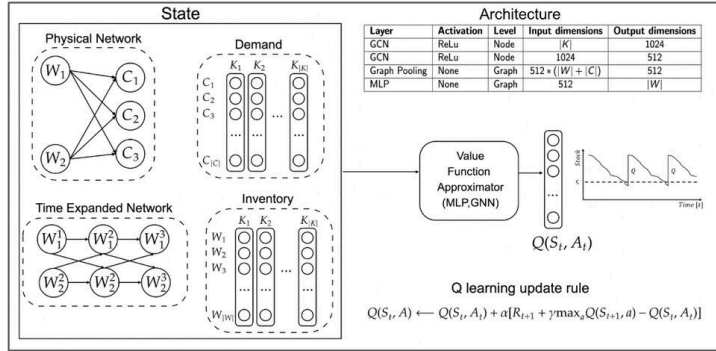


### Explainable Process Prediction

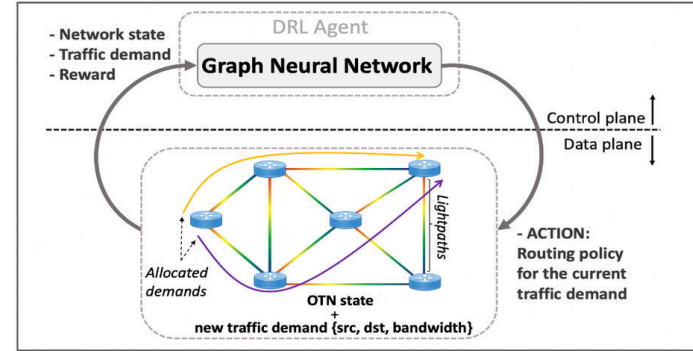


## Graph Neural Networks with Reinforcement Learning

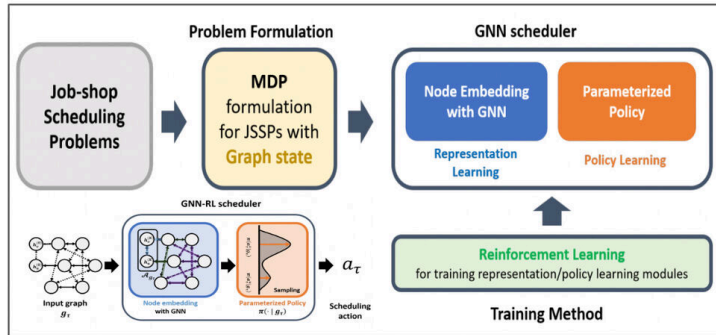
### Multi-Echelon Inventory Optimization



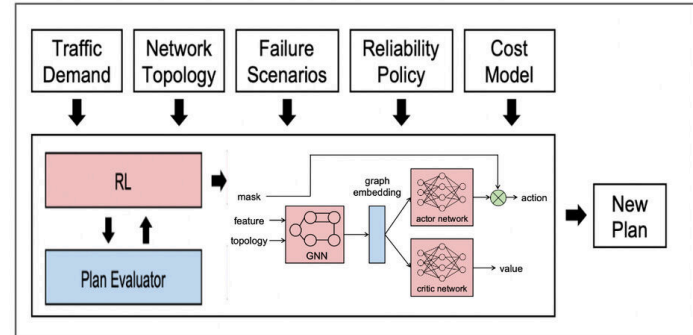
### Logistics, Routing and Transportation



### Manufacturing Control and Scheduling



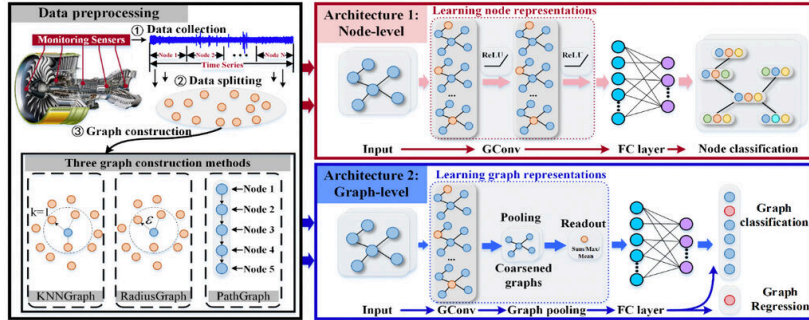
### Dynamic Network Control and Planning



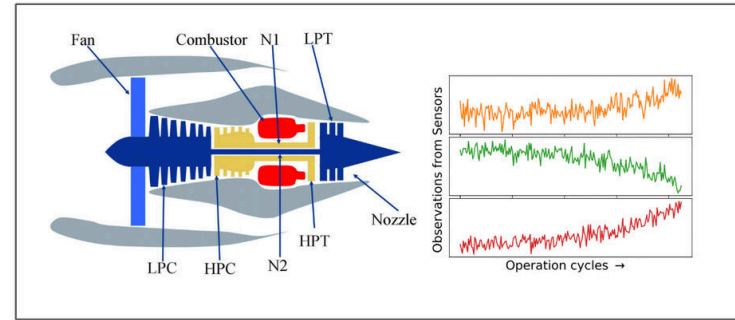
# 5ni. Производство

## Graph Neural Networks for Equipment Health Monitoring

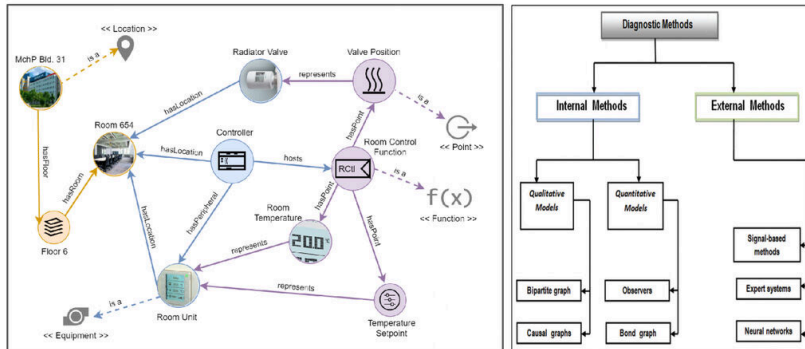
### Prognostics & Health Management, Fault Detection



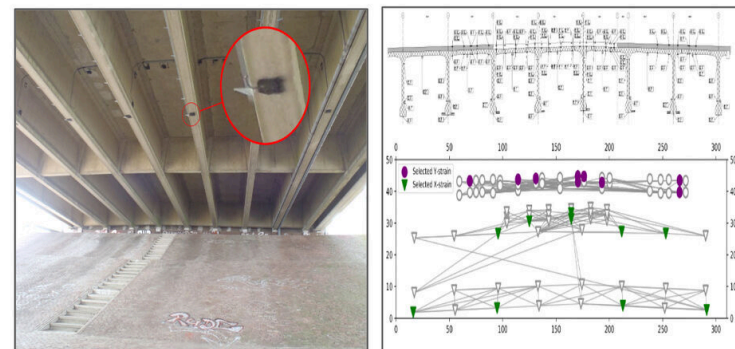
### Remaining Useful Lifetime Estimation, Anomaly Detection



### Semantic and Causal Condition Monitoring

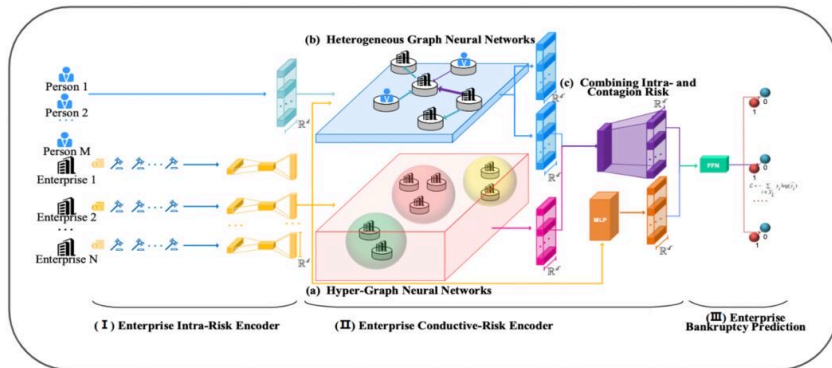


### Structural Health Monitoring

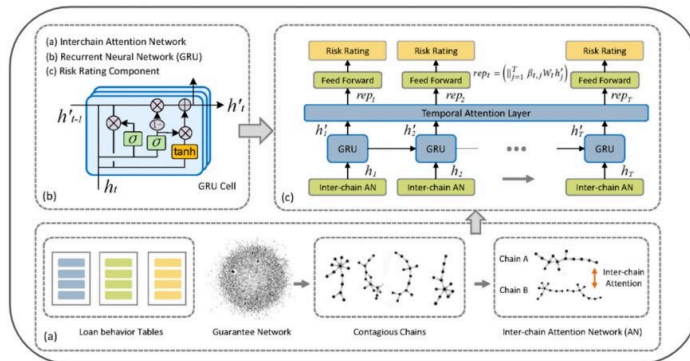




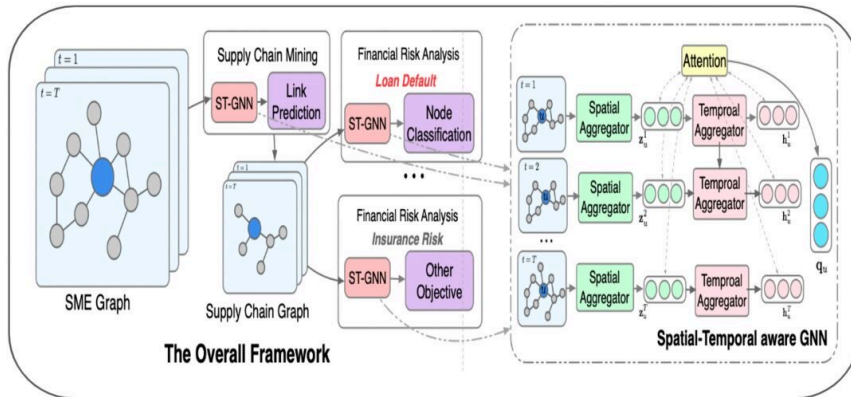
### Bankruptcy, Stock, Financial Event Prediction



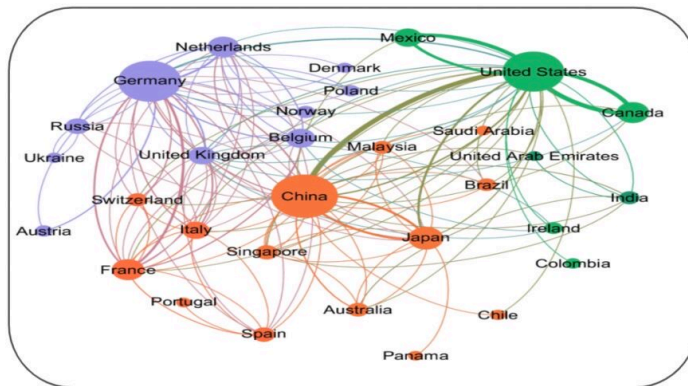
### System Risk & Stress Testing



### Supply Chain Risk Assessment



### International Trade Modeling - Gravity Models



# Перспективные направления исследований

02

## 2. Перспективные направления исследований



- Temporal graphs and Causality
- Uncertainty estimation
- Time-series prediction
- Explainability
- Large-scale (Kumo – 50 млрд вершин, etc.)
- Physics-Inspired Graph Neural Networks

**Physics-Inspired Graph Neural Networks (2023), M. Bronstein**

[https://www.youtube.com/watch?v=bb\\_JKLS8h4A](https://www.youtube.com/watch?v=bb_JKLS8h4A)

**Evaluating explainability for graph neural networks (2023)**

<https://www.nature.com/articles/s41597-023-01974-x>

# Современный стек в графах

03



### 3. Современный стек в графах



PyTorch  
geometric

[https://github.com/pyg-team/pytorch\\_geometric](https://github.com/pyg-team/pytorch_geometric)

<https://pytorch-geometric.readthedocs.io/en/latest/>



Torch  
Spatiotemporal

<https://torch-spatiotemporal.readthedocs.io/en/latest/>

<https://github.com/TorchSpatiotemporal/tsl>

Для распределенного обучения

graph-learn

 Alibaba.com

<https://github.com/alibaba/graphlearn-for-pytorch>

### 3. 23 ноября 2023



<https://github.com/MobileTeleSystems/CoolGraph>

- Легкий старт с GNN
- Автоподбор почти всего, в тч параметров предобработки данных, размера батча, архитектур, параметров слоев и функций активации
- Поддерживает фичи вершин, ребер, группы вершин с разными наборами фичей
- Эксперименты трекаются в MLFlow
- Можно использовать для быстрого получения эмбединга

# 3. последний релиз 15 августа 2023



<https://github.com/dmlc/dgl>

amazon.com

## 📌 Important Announcement: Deprecation of MXNet and TensorFlow Support in DGL 2.0

■ Questions



frozenbugs

Aug 23

📢 Important DGL Update: After DGL 2.0 (ETA: 2023Q4), we'll be prioritizing PyTorch backend due to resource constraints, saying goodbye to MXNet and TensorFlow support. Don't worry though – if you still need them, you can use older DGL versions. We're here to help you transition smoothly. Thanks for your understanding and ongoing support!

Aug 23

1 / 2

Aug 23

# Базовые операции и приемы

04

# Pipeline



01

02

03

Индексация,  
семплинг,  
трансформации  
фичей,  
маскирование и  
пр.  
– на семинаре



Батчи и  
нормализация  
– на семинаре



Message  
Passing

# Graph neural networks: a review of methods and applications (2020)

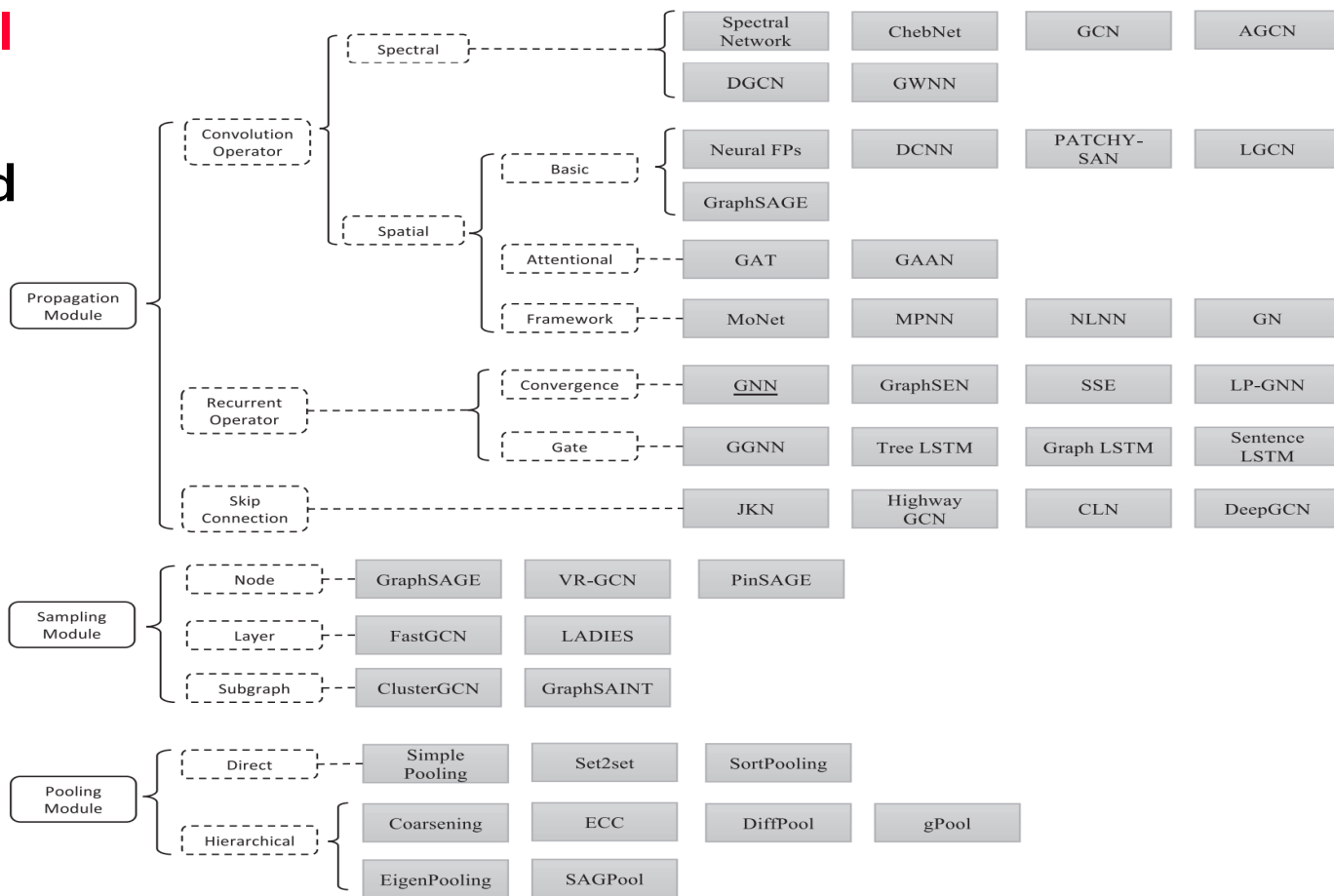


Fig. 3. An overview of computational modules.

## 14. Социальные сети и СМИ

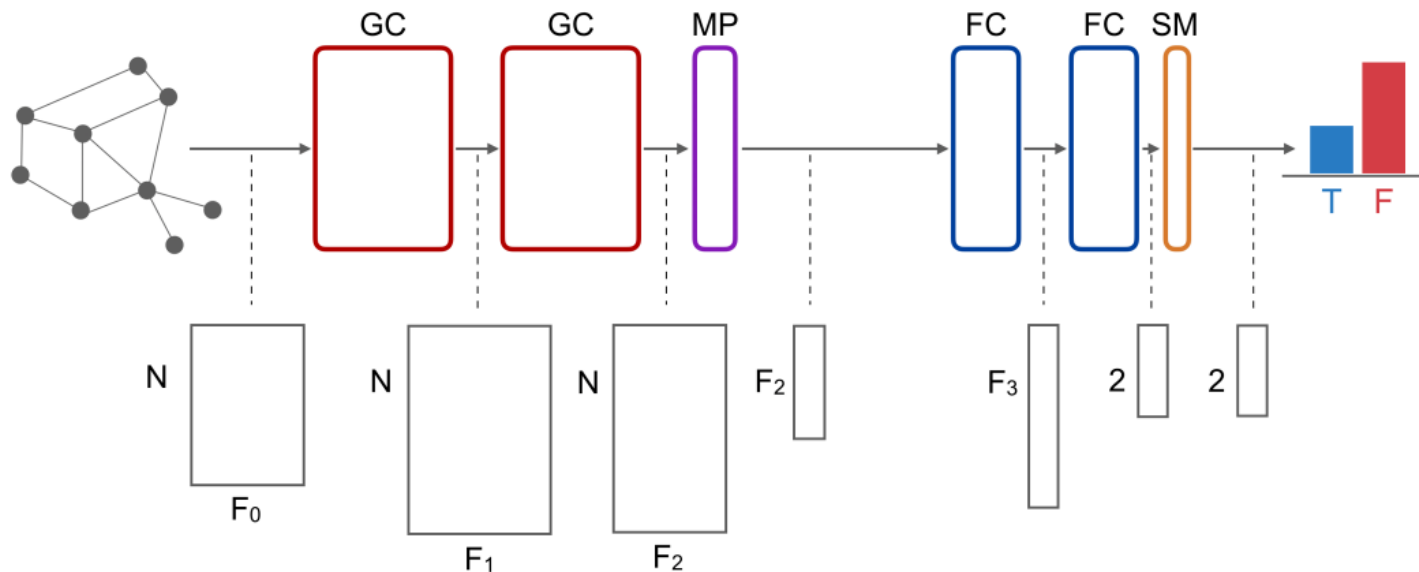


Figure 5: The architecture of our neural network model. Top row: GC = Graph Convolution, MP = Mean Pooling, FC = Fully Connected, SM = SoftMax layer. Bottom row: input/output tensors received/produced by each layer.

Fake News Detection on Social Media using Geometric Deep Learning (2019)

<https://arxiv.org/pdf/1902.06673.pdf>

# Графовая свертка GraphConv



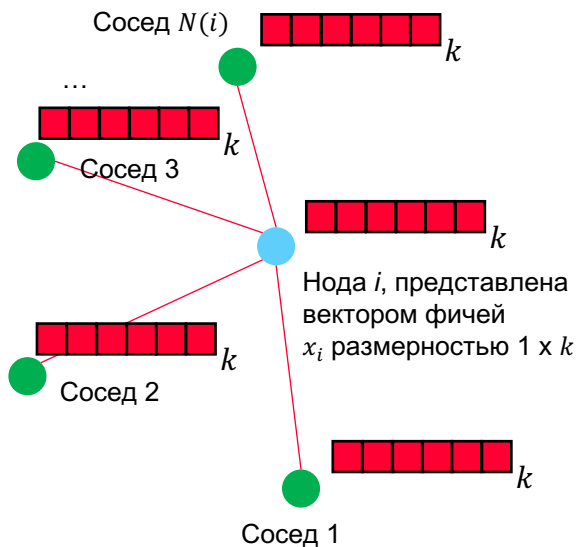
Нода  $i$ , представлена  
вектором фичей  
 $x_i$  размерностью  $1 \times k$

[https://pytorch-geometric.readthedocs.io/en/latest/generated/torch\\_geometric.nn.conv.GraphConv.html](https://pytorch-geometric.readthedocs.io/en/latest/generated/torch_geometric.nn.conv.GraphConv.html)

<https://arxiv.org/pdf/1704.01212.pdf>  
<https://arxiv.org/pdf/1810.02244.pdf>  
<https://arxiv.org/pdf/1709.05584.pdf>



# Графовая свертка GraphConv



[https://pytorch-geometric.readthedocs.io/en/latest/generated/torch\\_geometric.nn.conv.GraphConv.html](https://pytorch-geometric.readthedocs.io/en/latest/generated/torch_geometric.nn.conv.GraphConv.html)

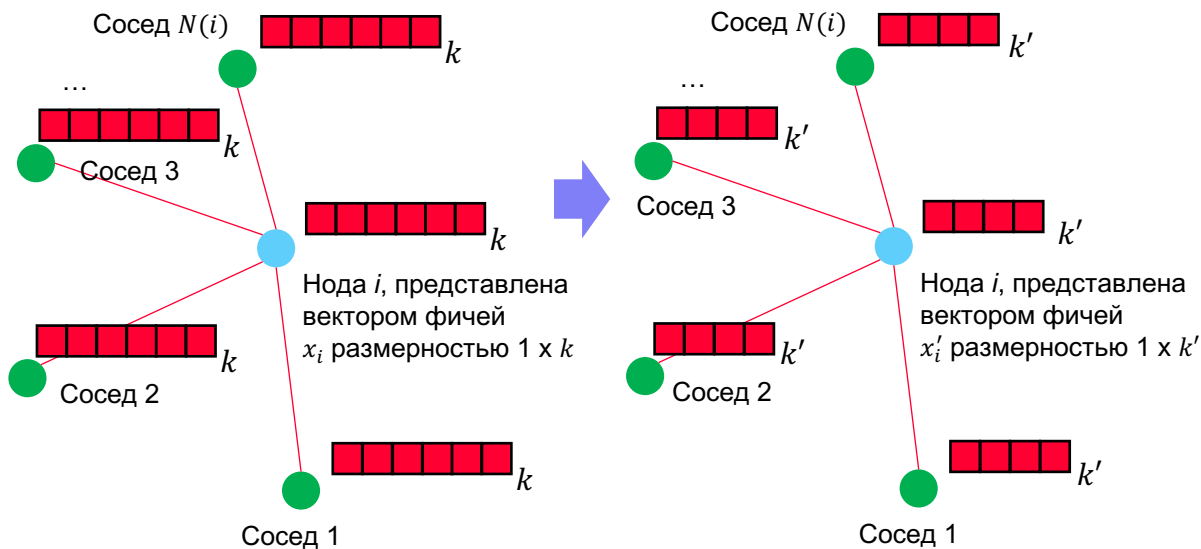
<https://arxiv.org/pdf/1704.01212.pdf>  
<https://arxiv.org/pdf/1810.02244.pdf>  
<https://arxiv.org/pdf/1709.05584.pdf>

# Графовая свертка GraphConv

$$x'_i = Hx_i + \sum_{j \in [1, N(i)]} Wx_j$$

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$W$  и  $H$  имеют размерность  $k \times k'$ :  
 $(1 \times k) * (k \times k') = 1 \times k'$



[https://pytorch-geometric.readthedocs.io/en/latest/generated/torch\\_geometric.nn.conv.GraphConv.html](https://pytorch-geometric.readthedocs.io/en/latest/generated/torch_geometric.nn.conv.GraphConv.html)

<https://arxiv.org/pdf/1704.01212.pdf>

<https://arxiv.org/pdf/1810.02244.pdf>

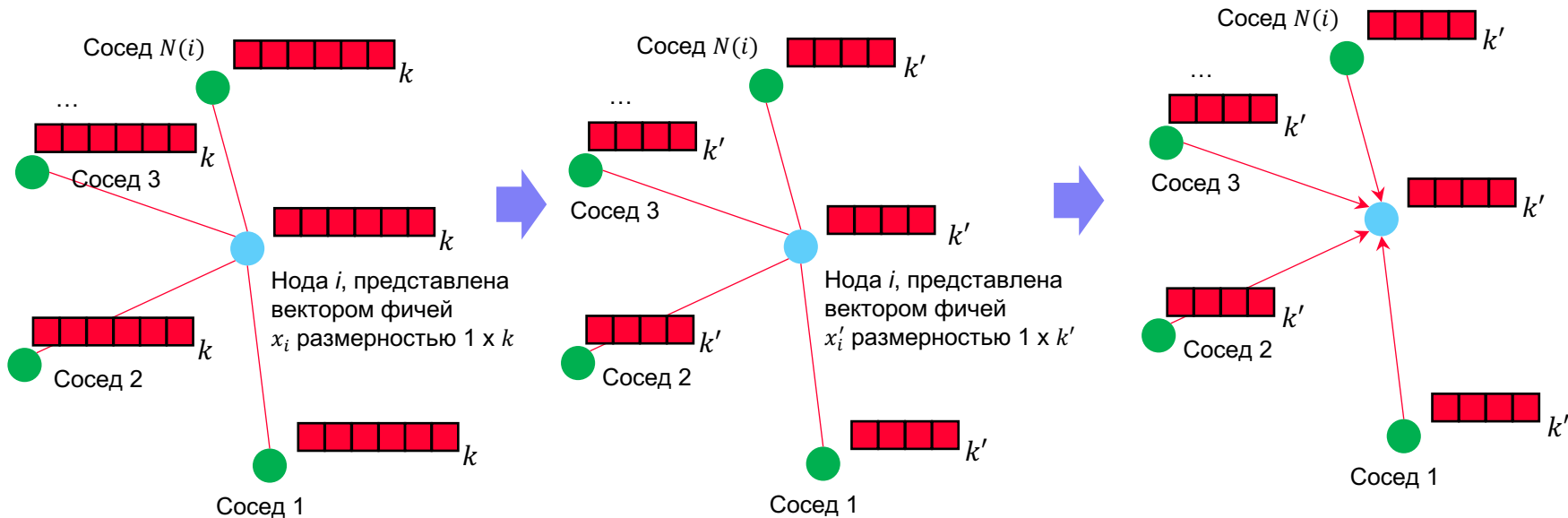
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<https://arxiv.org/pdf/1704.01212.pdf>

<https://arxiv.org/pdf/1810.02244.pdf>

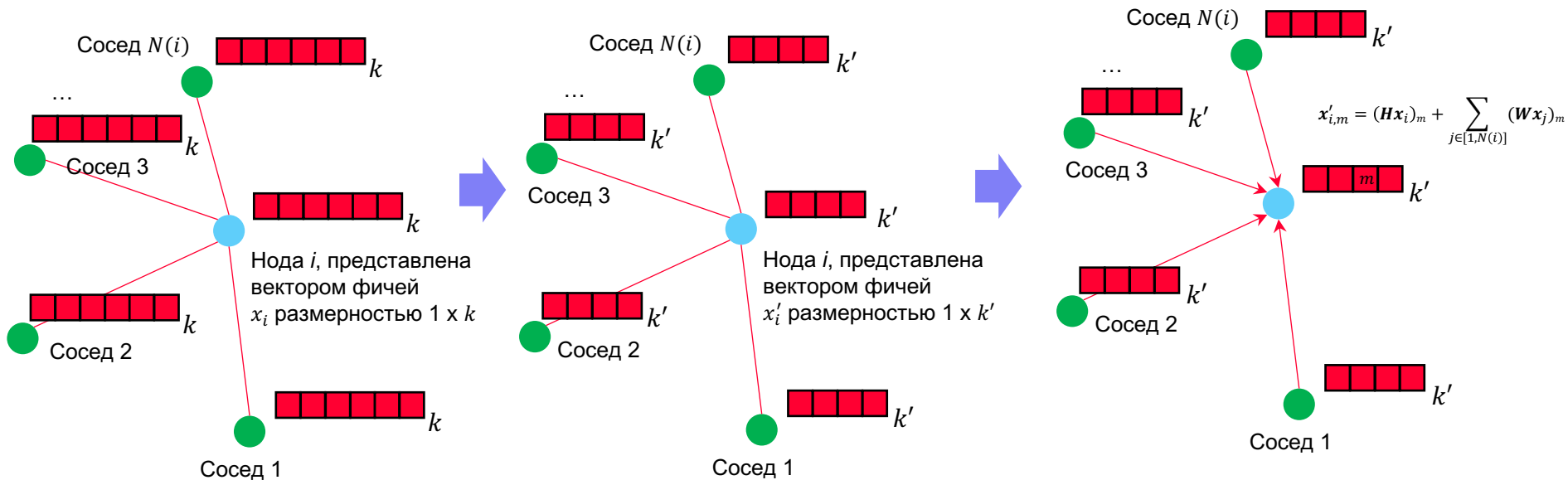
<https://arxiv.org/pdf/1709.05584.pdf>

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<https://arxiv.org/pdf/1704.01212.pdf>

<https://arxiv.org/pdf/1810.02244.pdf>

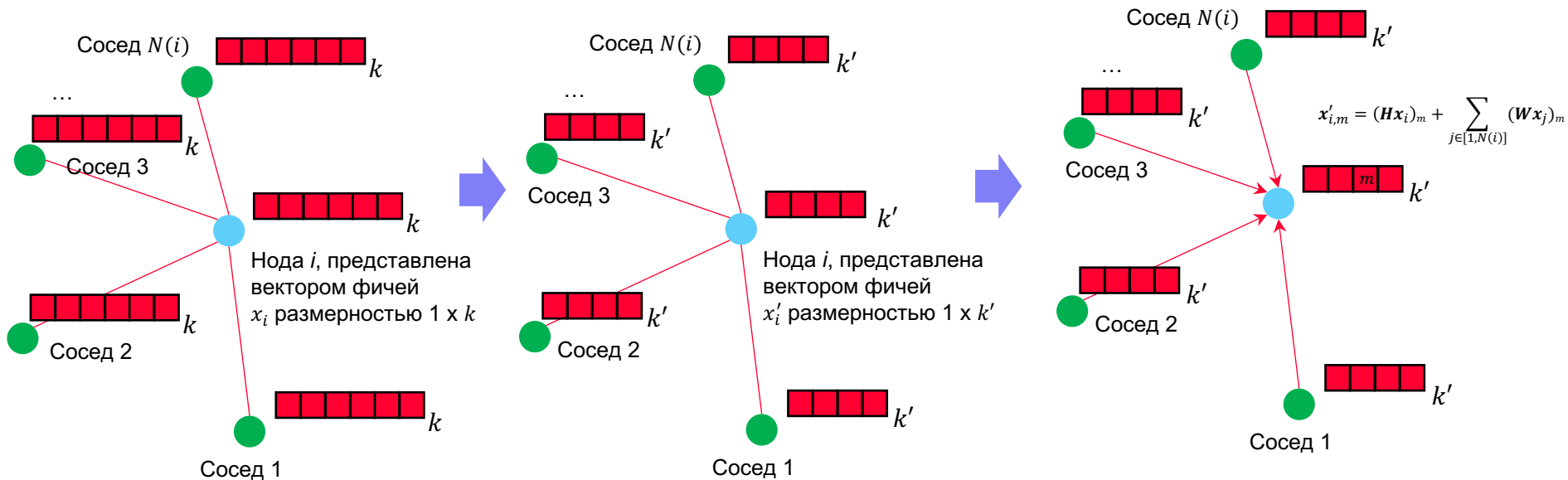
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[https://pytorch-geometric.readthedocs.io/en/latest/generated/torch\\_geometric.nn.conv.GraphConv.html](https://pytorch-geometric.readthedocs.io/en/latest/generated/torch_geometric.nn.conv.GraphConv.html)

Вместо суммы – другие агрегирующие функции

<https://arxiv.org/pdf/1704.01212.pdf>

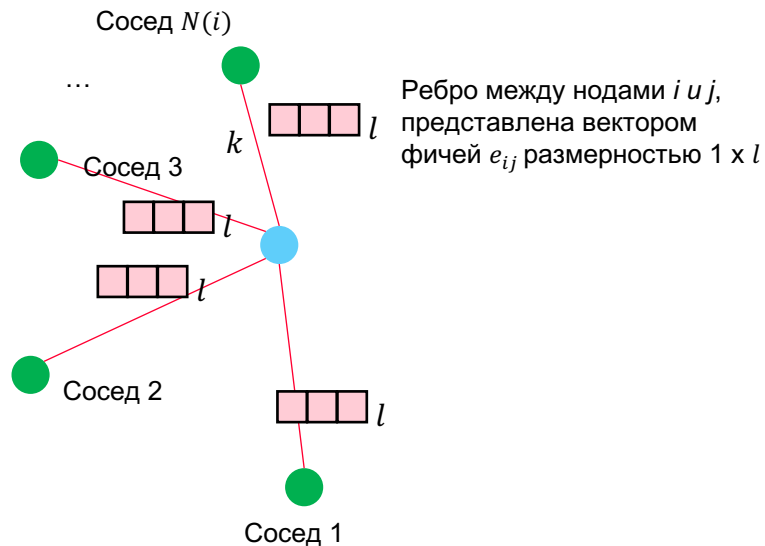
<https://arxiv.org/pdf/1810.02244.pdf>

<https://arxiv.org/pdf/1709.05584.pdf>

# Графовая свертка NNConv



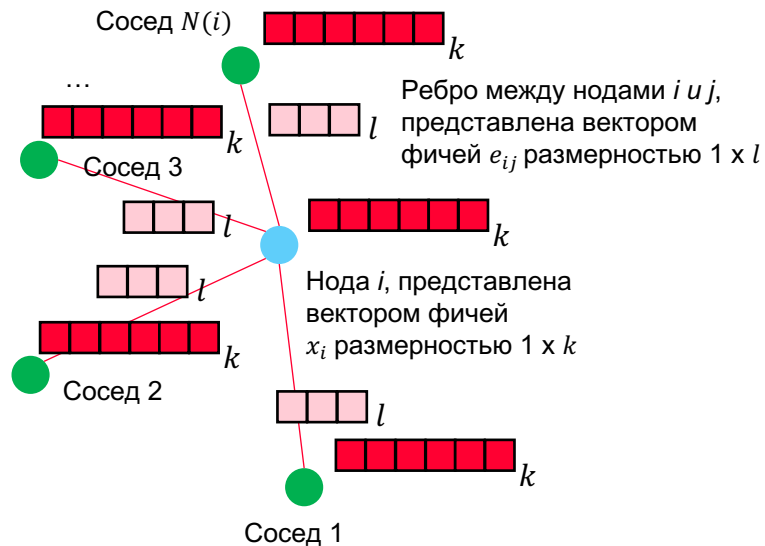
$$\mathbf{x}'_i = \mathbf{H}\mathbf{x}_i + \sum_{j \in [1, N(i)]} \mathbf{x}_j \text{NN}(\mathbf{e}_{ij})$$



# Графовая свертка NNConv



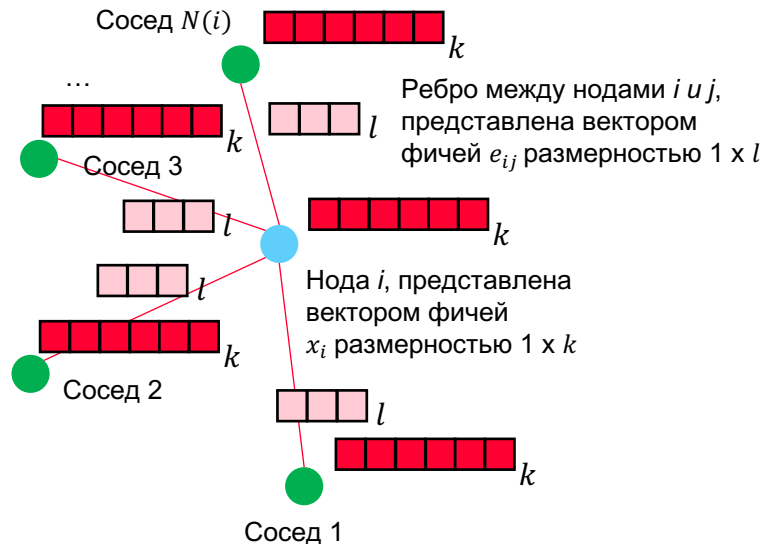
$$x'_i = Hx_i + \sum_{j \in [1, N(i)]} x_j NN(e_{ij})$$



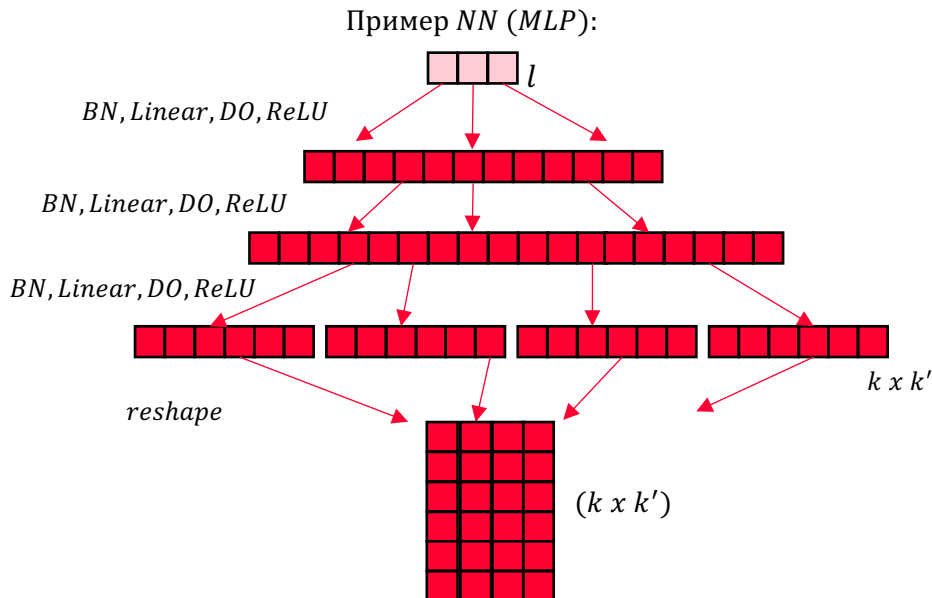
# Графовая свертка NNConv



$$x'_i = Hx_i + \sum_{j \in [1, N(i)]} x_j NN(e_{ij})$$



$H$  и выходной слой  $NN$  имеют размерность  $k \times k'$ :  
 $(1 \times k) * (k \times k') = 1 \times k'$   
Входной слой  $NN$  имеет размерность  $l$   
( $NN$  — часто  $MLP$ )



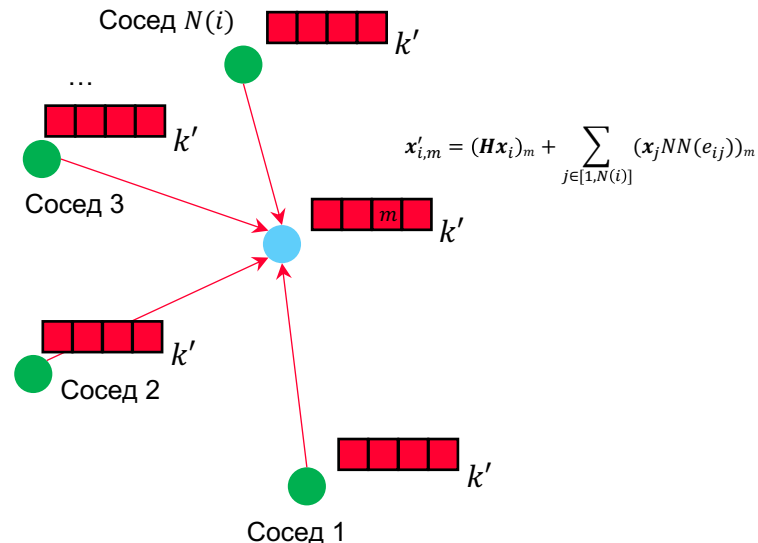
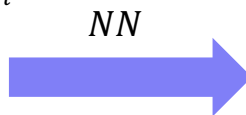
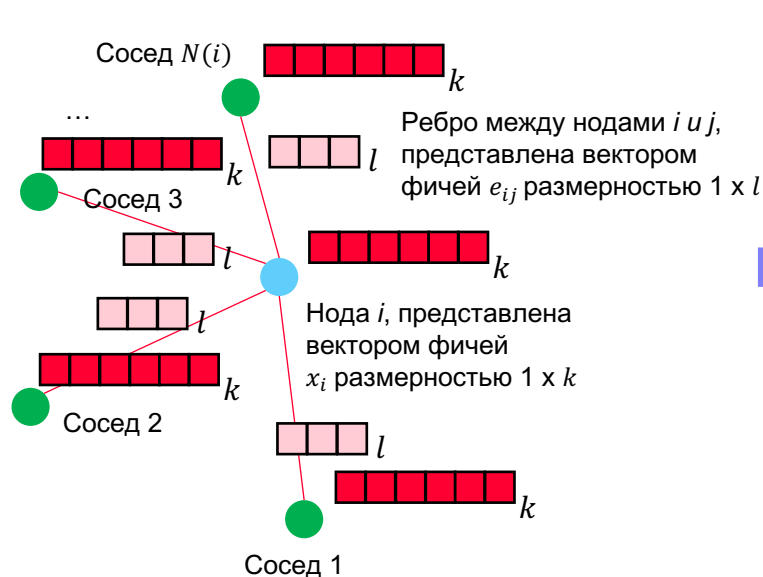


# Графовая свертка NNConv

$k'$

$$x'_i = Hx_i + \sum_{j \in [1, N(i)]} x_j NN(e_{ij})$$

$H$  и выходной слой  $NN$  имеют размерность  $k \times k'$ :  
 $(1 \times k) * (k \times k') = 1 \times k'$   
 Входной слой  $NN$  имеет размерность  $l$   
 ( $NN$  — часто  $MLP$ )



Где брать  
актуальную  
информацию:  
полезные ресурсы и  
персоналии

05

# Персоналии



Проф. Михаил Бронштейн  
DeepMind Professor of AI,  
University of Oxford

<https://www.cs.ox.ac.uk/people/michael.bronstein/>



Prof. Jure Leskovec

<http://snap.stanford.edu/people.html>



Михаил Галкин

<https://migalkin.github.io/>

# Курсы по GNN



**Penn, Graph  
Neural Networks**

<https://gnn.seas.upenn.edu/lectures/>



**Weights and  
biases, ML with  
Graphs**

<https://wandb.ai/sylogismos/machine-learning-with-graphs/reports/1-Introduction-Structure-of-Graphs--VmlldzozNzU1NDU>



**Stanford / Fall  
2023, CS224W:  
Machine Learning  
with Graphs**

<http://web.stanford.edu/class/cs224w/>

# Семинары и конференции



Temporal Graph Learning Workshop @ NeurIPS 2023

<https://sites.google.com/view/tglworkshop-2023/home>

New Frontiers in Graph Learning, Workshop @ NeurIPS 2022

<https://nips.cc/virtual/2022/workshop/49963>



STANFORD

Stanford Graph Learning Workshop

<https://snap.stanford.edu/graphlearning-workshop-2023/>



RecSys, графовая секция

<https://recsys.acm.org/recsys23/session-6/>

ICCV23  
PARIS

1st Workshop on Scene Graphs and Graph Representation Learning

<https://openaccess.thecvf.com/ICCV2023/workshops/SG2RL>



3 семинара по обучению на графах

<https://kdd.org/kdd2023/workshops/>

# Ресурсы и датасеты

## Почитать



<https://dl.acm.org/doi/10.1145/3580305.3599207>



Papers With Code

<https://paperswithcode.com/>



Robust reasoning over Knowledge Graph with LLM  
<https://github.com/RManLuo/Awesome-LLM-KG>



[tg: @graphML](https://t.me/graphML)

## Датасеты



<https://docs.dgl.ai/api/python/dgl.data.html#fraud-dataset>



<https://pytorch-geometric.readthedocs.io/en/latest/modules/datasets.html>