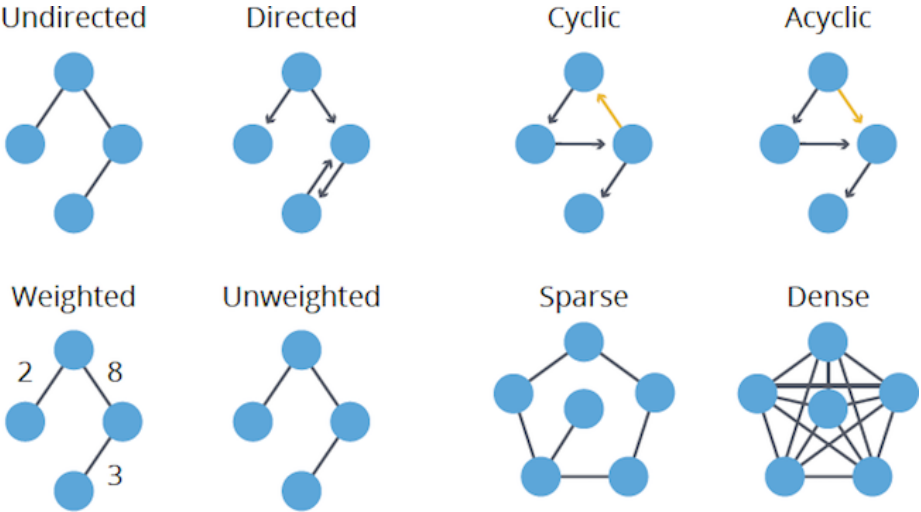
Глубокое обучение и вообще

Кирпа Вадим

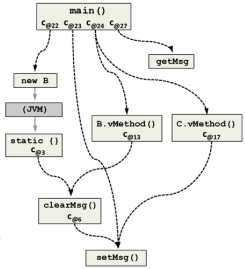
1 февраля 2023 г.

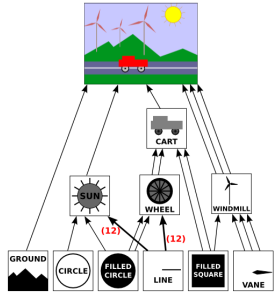
Графовые нейронные сети

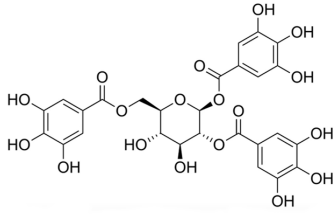
Графы


Undirected
Directed
Cyclic
Acyclic
Weighted
2
8
3
Unweighted
Sparse
Dense

Графы в жизни







Картинки как графы

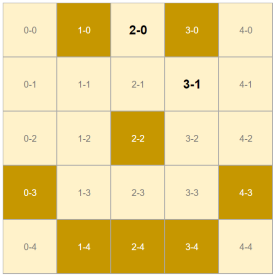
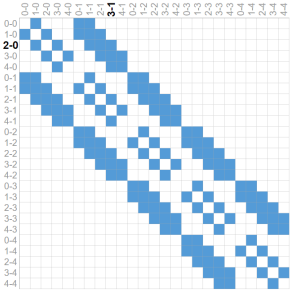
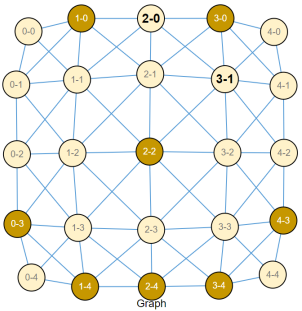


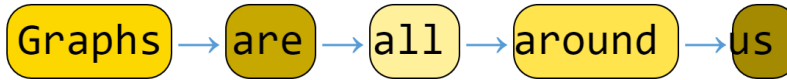
Image Pixels

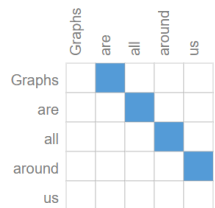

Adjacency Matrix



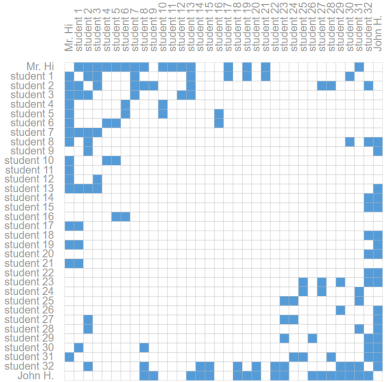
Graph

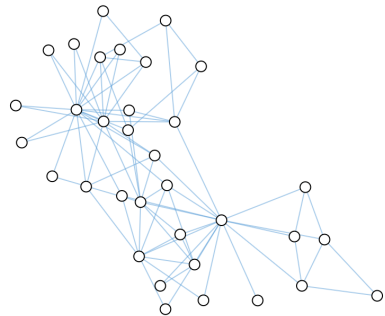
Текст как графы



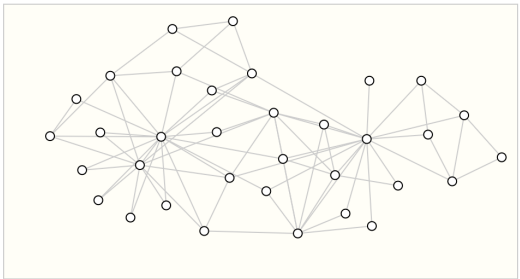


Пример графа

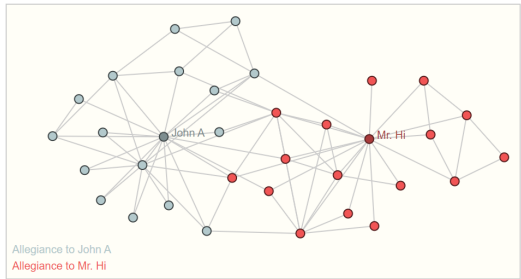




Задачи на графах: вершины



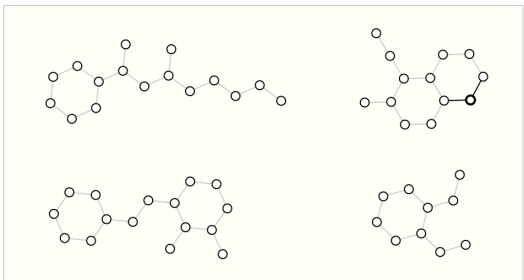
→



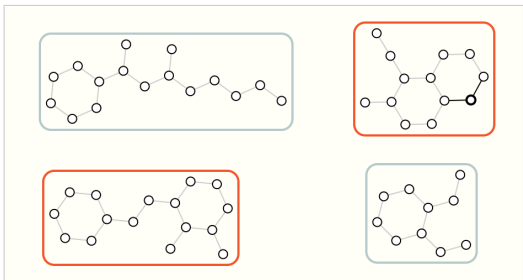
Input: graph with unlabled nodes

Output: graph node labels

Задачи на графах: целый граф

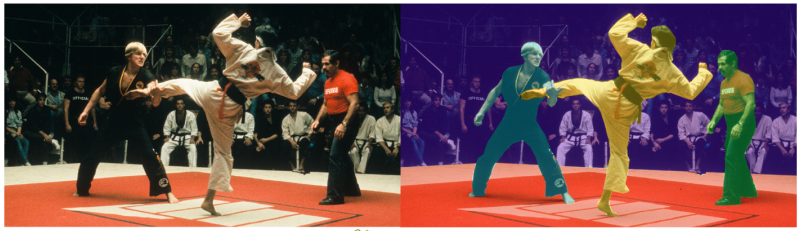


Input: graphs

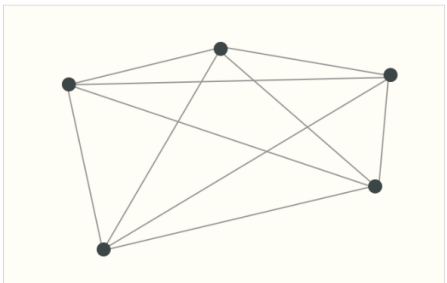


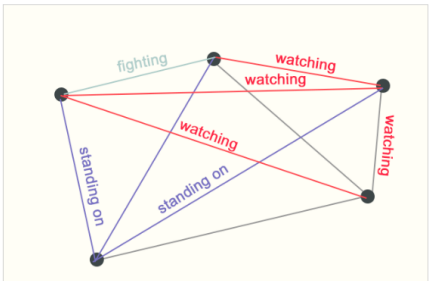
Output: labels for each graph, (e.g., "does the graph contain two rings?")

Задачи на графах: ребра



Задачи на графах: ребра





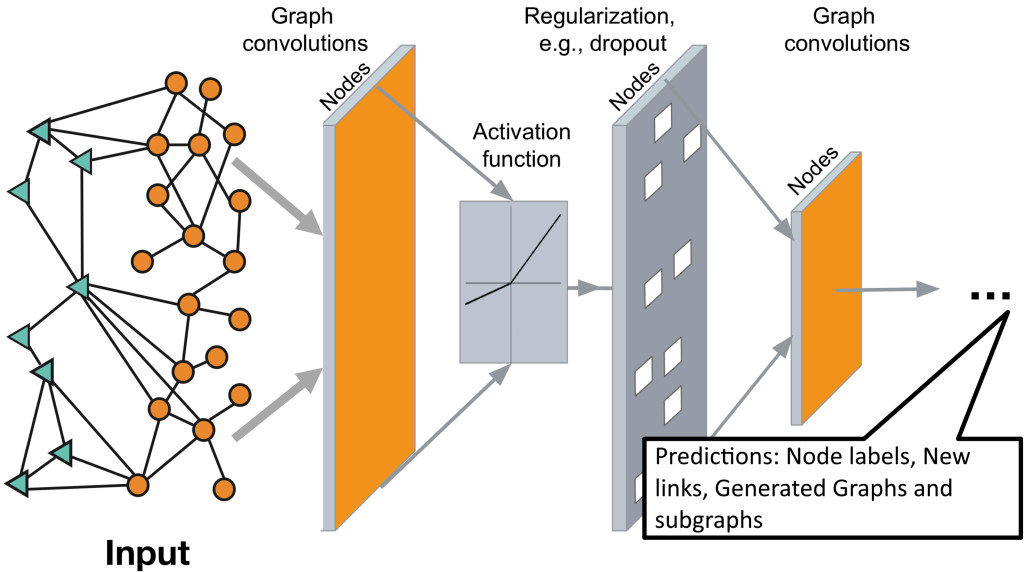
Input: fully connected graph, unlabeled edges

Output: labels for edges

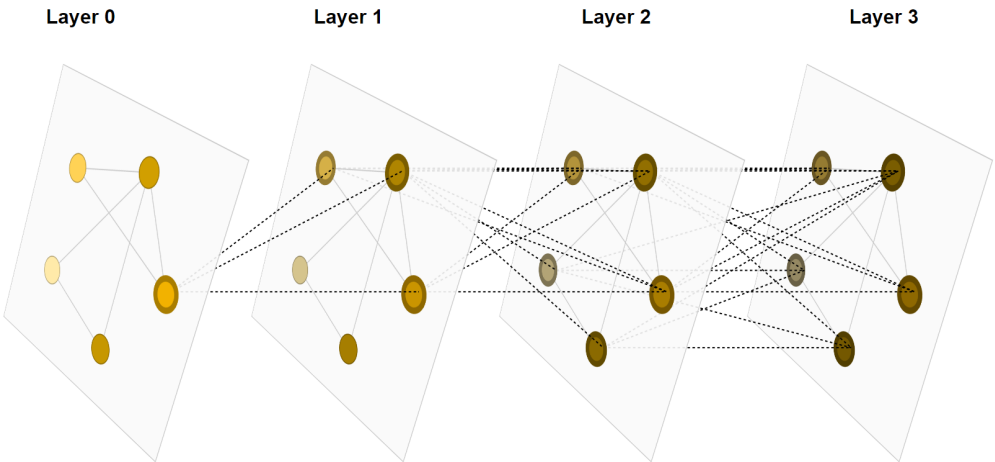
Проблемы при работу с графами

- Размеры
- Часто имеют динамическую структуру
- Нет порядка вершин

Графы


Graph convolutions
Nodes
Activation function
Regularization, e.g., dropout
Nodes
Graph convolutions
Nodes
...
Predictions: Node labels, New links, Generated Graphs and subgraphs
Input

Message Passing



GraphSAGE

Algorithm 1: GraphSAGE embedding generation (i.e., forward propagation) algorithm

Input : Graph $\mathcal{G}(\mathcal{V}, \mathcal{E})$; input features $\{\mathbf{x}_v, \forall v \in \mathcal{V}\}$; depth K; weight matrices $\mathbf{W}^k, \forall k \in \{1, ..., K\}$; non-linearity σ; differentiable aggregator functions $\text{AGGREGATE}_k, \forall k \in \{1, ..., K\}$; neighborhood function $\mathcal{N} : v \rightarrow 2^{\mathcal{V}}$

Output : Vector representations $\mathbf{z}_v$ for all $v \in \mathcal{V}$

$\mathbf{h}_v^0 \leftarrow \mathbf{x}_v, \forall v \in \mathcal{V}$;
for $k = 1...K$ **do**
  for $v \in \mathcal{V}$ **do**
    $\mathbf{h}_{\mathcal{N}(v)}^k \leftarrow \text{AGGREGATE}_k(\{\mathbf{h}_u^{k-1}, \forall u \in \mathcal{N}(v)\})$;
    $\mathbf{h}_v^k \leftarrow \sigma\left(\mathbf{W}^k \cdot \text{CONCAT}(\mathbf{h}_v^{k-1}, \mathbf{h}_{\mathcal{N}(v)}^k)\right)$
  end
  $\mathbf{h}_v^k \leftarrow \mathbf{h}_v^k / \|\mathbf{h}_v^k\|_2, \forall v \in \mathcal{V}$
end
$\mathbf{z}_v \leftarrow \mathbf{h}_v^K, \forall v \in \mathcal{V}$

Почитать

- Graph Convolution Network: https://arxiv.org/pdf/1609.02907.pdf
- GraphSAGE: https://arxiv.org/pdf/1706.02216.pdf
- Graph Attention Network: https://arxiv.org/pdf/1710.10903.pdf
- Overview: https://arxiv.org/pdf/1810.00826.pdf