

Graph Neural Network

Einführung in GNNs

Tin Votan, 16. März 2021

Einführung

Blabla ...

- Graph neural networks (GNNs) are proposed to combine the feature information and the graph structure to learn better representations on graphs via feature propagation and aggregation. Due to its convincing performance and high interpretability, GNN has recently become a widely applied graph analysis tool.
- Graph neural networks (GNNs) are deep learning-based methods that operate on graph domain. Due to its convincing performance and high interpretability, GNN has been a widely applied graph analysis method recently.

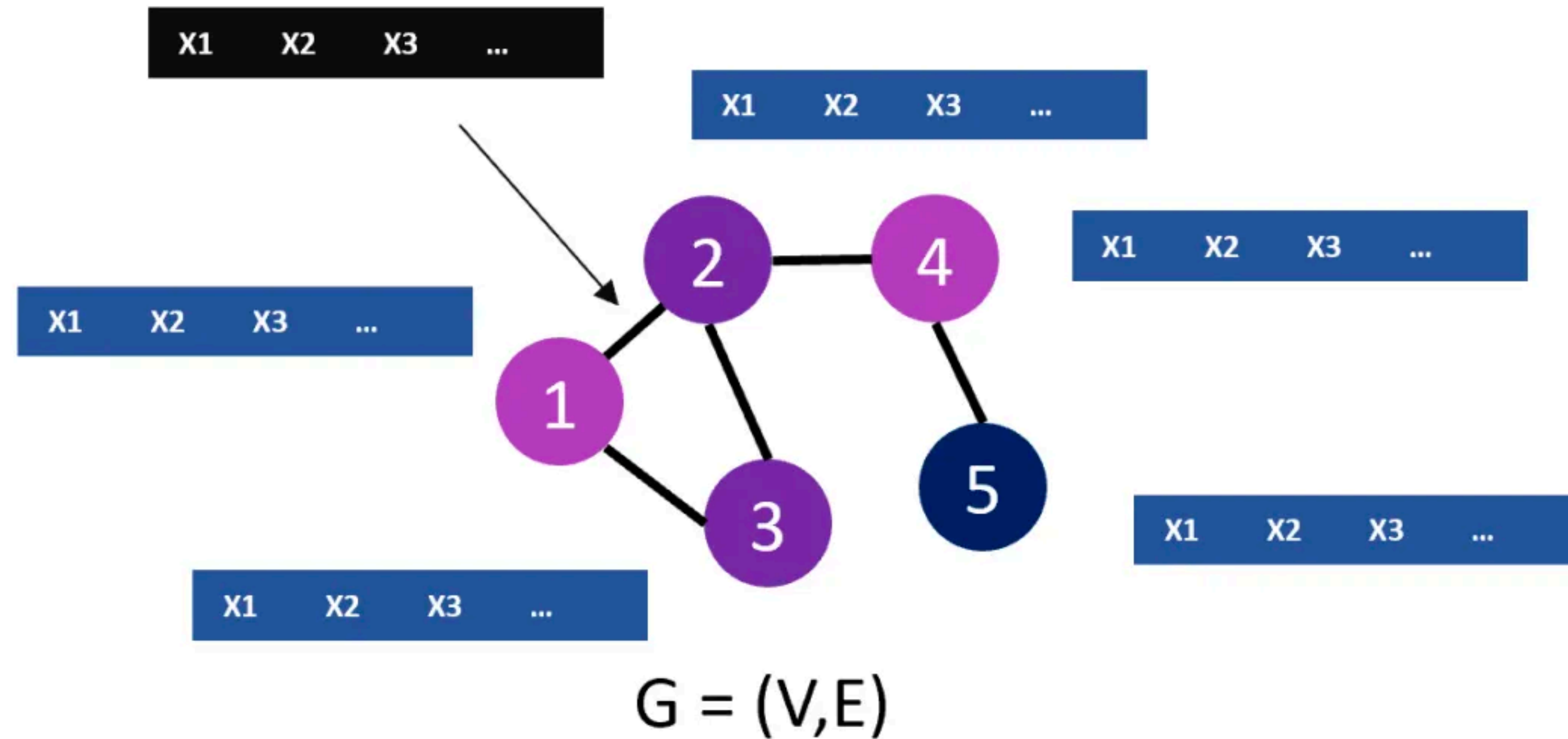
- Formel:

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

The diagram illustrates the components of the GNN formula. It shows three input representations: a single row vector $[x_1, x_2, x_3, \dots]$ with x_3 highlighted in orange, another single row vector $[x_1, x_2, x_3, \dots]$ with x_3 highlighted in orange, and a 3x4 matrix of blue blocks. Arrows point from the first two vectors to the $\text{UPDATE}^{(k)}$ function and from the matrix to the $\text{AGGREGATE}^{(k)}$ function. The $\text{AGGREGATE}^{(k)}$ function also receives a set of neighbor hidden states $\{h_v^{(k)} | v \in \mathcal{N}(u)\}$ as input.

Einführung

Ein einfacher Graph

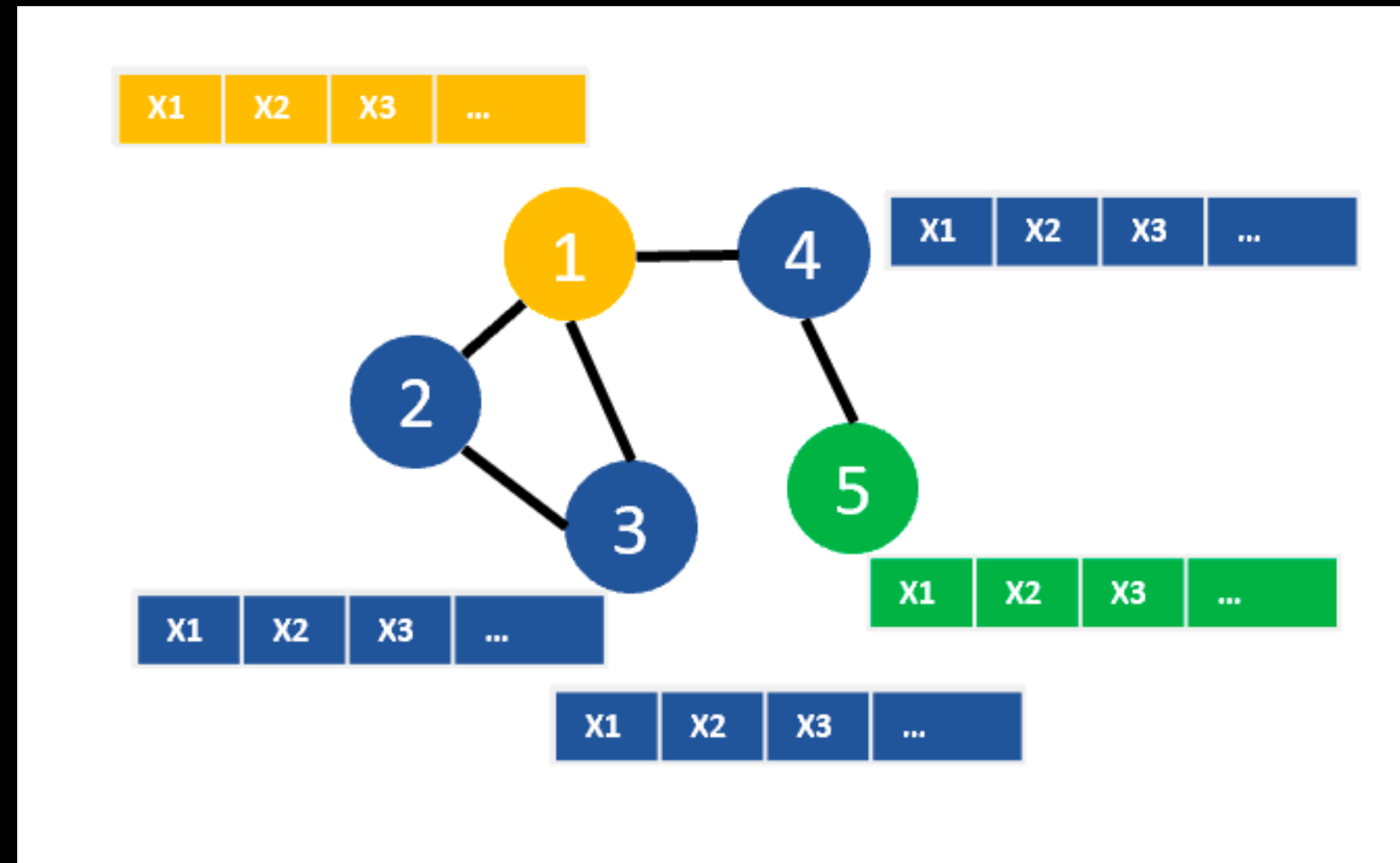


	V1	V2	...
V1	0	1	...
V2	1	0	...
V3	1	1	...
...

Adjacency matrix

Einführung

Nodes und Features



(Quelle: deepfindr.com)

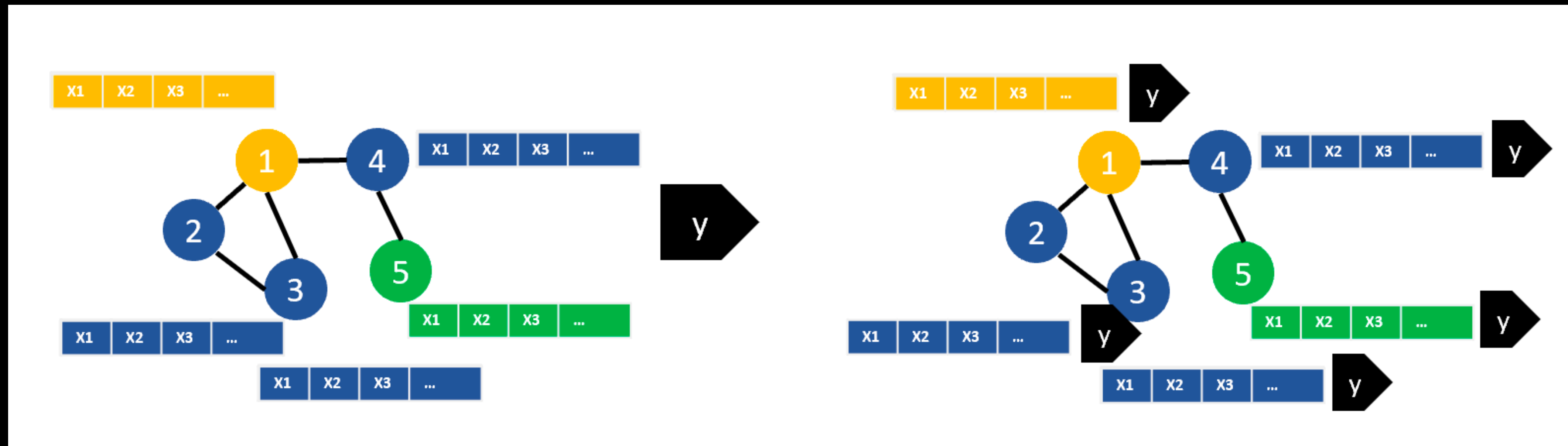
3 Verbindungen

2 Verbindungen

2 Verbindungen

Einführung

Nodes und Features

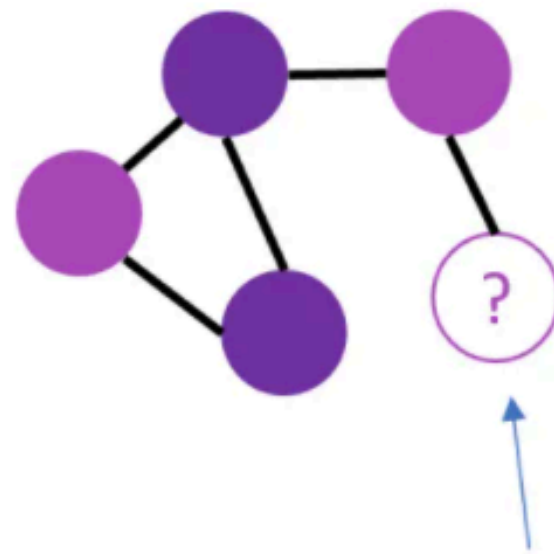


(Quelle: deepfindr.com)

Einführung

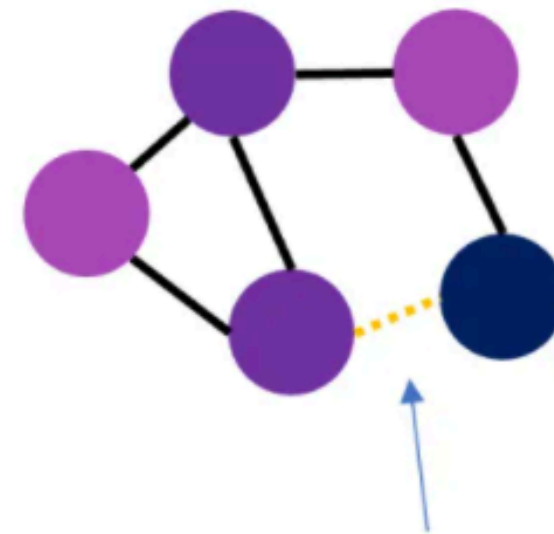
Beispiele zur Interpretation:

Node-level predictions



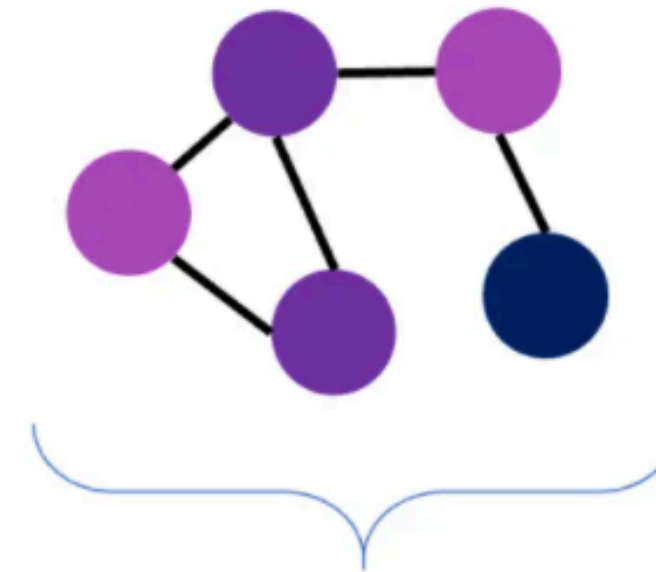
Does this person smoke?
(unlabeled node)

Link prediction (node pairs)



Next Netflix video?

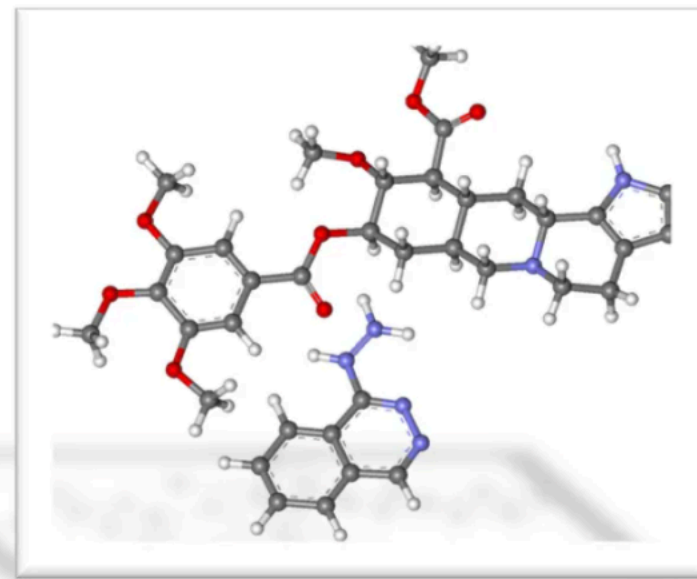
Graph-level predictions



Is this molecule a suitable drug?

Einführung

Einsatz in ...



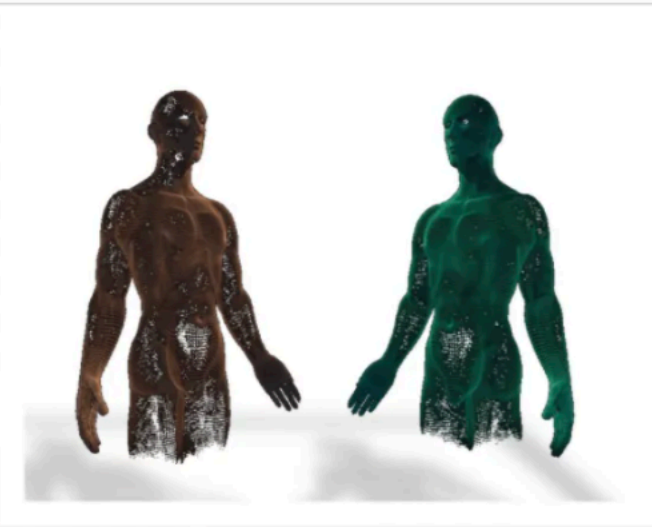
Medicine / Pharmacy



Recommender Systems



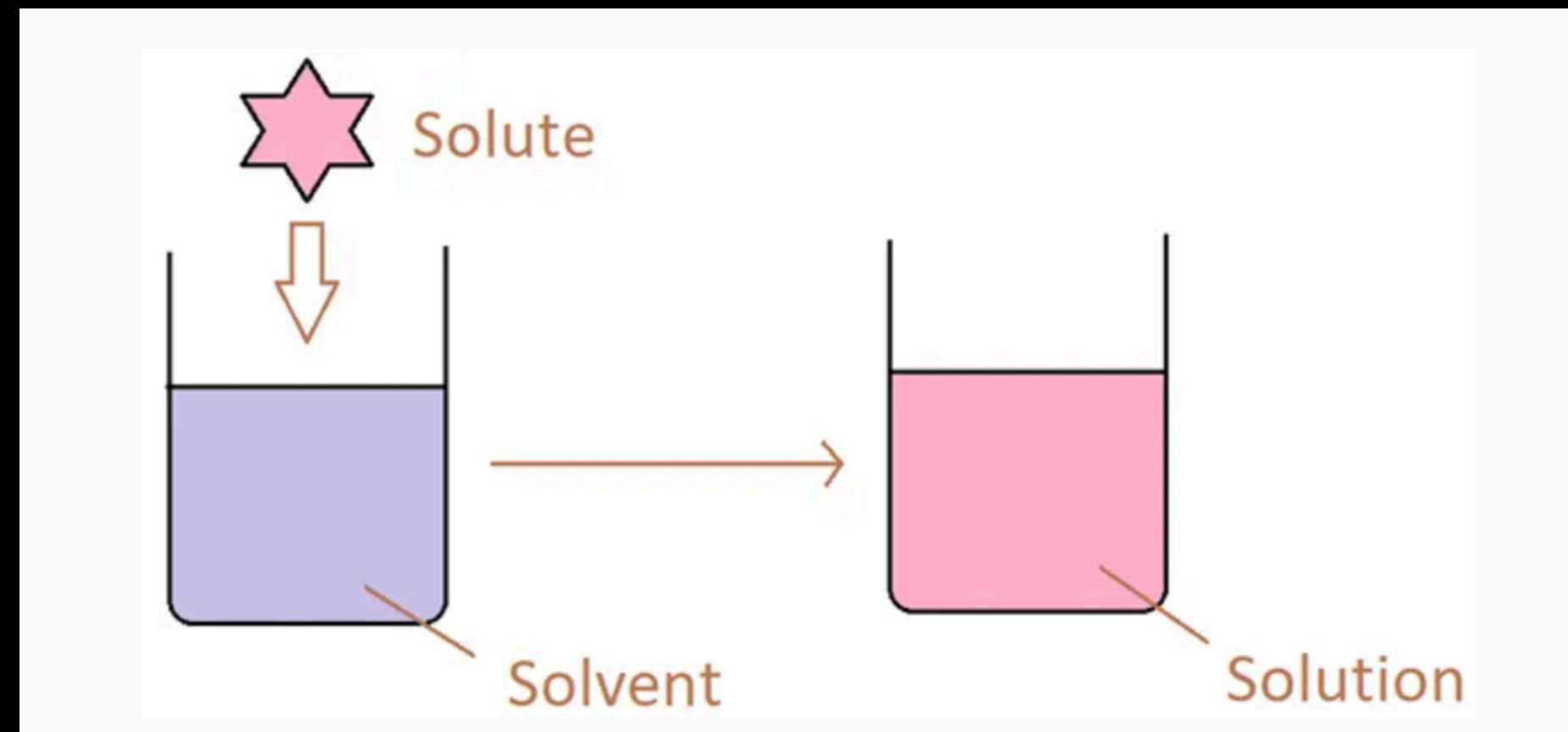
Social Networks



3D Games / Meshes

PyTorch Geometric

Kurz gesagt ...



“Unsere Machine Learning Aufgabe ist es vorherzusagen, wie sich verschiedene Moleküle in Wasser auflösen.”

Links

- <https://github.com/thunlp/GNNPapers>
- Introduction to Graph Neural Networks
(<https://doi.org/10.2200/S00980ED1V01Y202001AIM045>)
- <https://youtu.be/fOctJB4kVIM>
- <https://pytorch-geometric.readthedocs.io/en/latest/index.html>
- <https://medium.com/@sunitachoudhary103/generating-molecules-using-a-char-rnn-in-pytorch-16885fd9394b>
- <https://deepfindr.com/understanding-graph-neural-networks-part-1-3/>