

Simon Delarue¹, Thomas Bonald¹, Tiphaine Viard²

¹LTCI, TÉLÉCOM PARIS, INSTITUT POLYTECHNIQUE DE PARIS

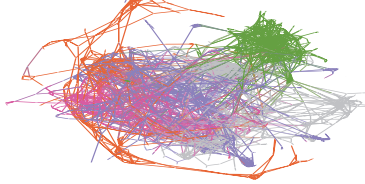
²LTCI / I3, TÉLÉCOM PARIS, INSTITUT POLYTECHNIQUE DE PARIS

- MOTIVATION

GRAPHS ARE EVERYWHERE



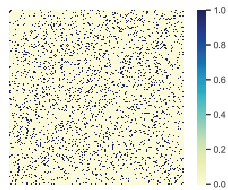
Graph of airplane traffic



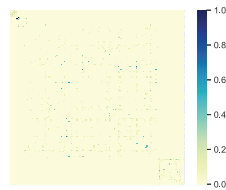
Graph of citations between scientific publications

REAL-WORLD GRAPHS ARE SPARSE

- In real-world graphs: $m \ll n^2$, with m the number of edges and n the number of nodes
- **Sparse format** encoding



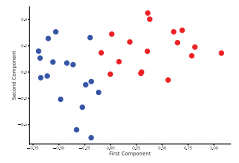
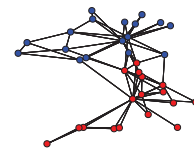
Dense random graph



Sparse real-world graph

REPRESENTATION LEARNING

- **Non-Euclidean** data structure
- Machine learning tasks: node classification, link prediction, etc.
- **Deep-learning** based approaches show great results^[1]

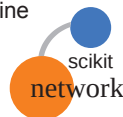


Embedding of Karate-club graph

- Graph Neural Networks in Scikit-network

SCIKIT-NETWORK^[2]

- Python package for **machine learning on graphs**
- **Performant** and **easy** to use:
 - Based on efficient sparse graph representation
 - Reproduces Scikit-learn^[3] `fit_transform()` pipeline
- Real-world graph algorithms: clustering, ranking, embedding, visualisation, etc.

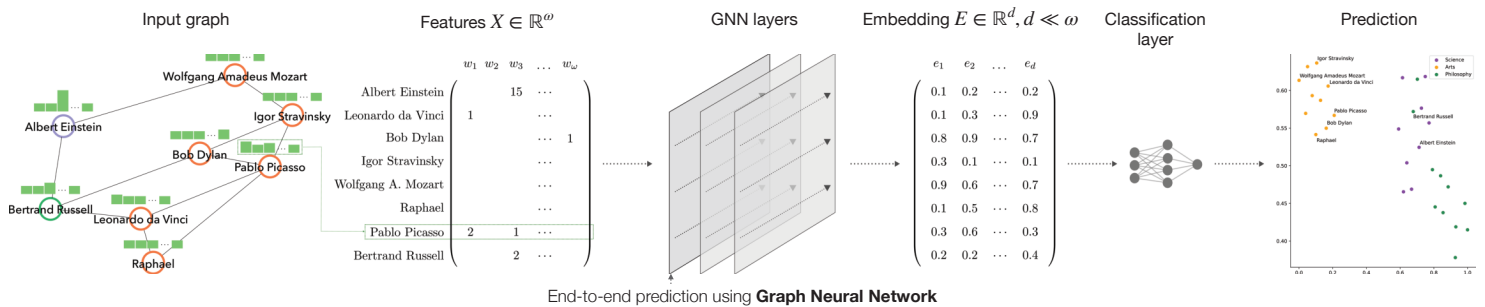


GRAPH NEURAL NETWORKS

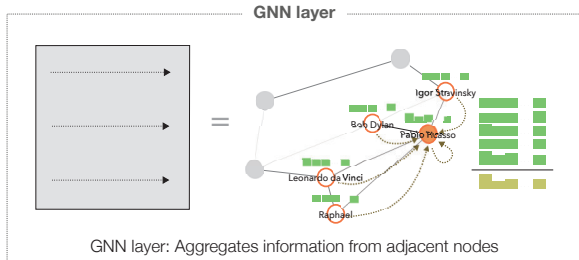
- **Graph Neural Networks (GNN)** approaches are extending neural networks to graph structures, in order to learn embeddings
- **Gather** and **aggregate** information

$$H^{(l+1)} = \sigma(\tilde{A}H^{(l)}W^{(l)} + b^{(l)})$$

APPLICATIONS



End-to-end prediction using Graph Neural Network



- **Enriched graphs** can provide valuable insights
- **Interdisciplinary** applications: perspectives between computer sciences and the social sciences
- Several remaining **challenges** about scalability, interpretability and fairness

- Contribution

- **Fast** and **scalable** implementation
- Reduce memory footprint thanks to **sparse formats**
- GNNs with **dependencies limited** to NumPy and SciPy

- References

[1] T. N. Kipf and M. Welling. Semi-Supervised Classification with Graph Convolutional Networks. In Proceedings of the 5th International Conference on Learning Representations, ICLR '17, 2017
 [2] T. Bonald, N. de Lara, Q. Lutz, and B. Charpentier. Scikit-network: Graph analysis in python. Journal of Machine Learning Research, 2020
 [3] F. Pedregosa, G. Varoquaux, A. Gramfort, V. Michel, B. Thirion, O. Grisel, M. Blondel, P. Prettenhofer, R. Weiss, V. Dubourg, J. Vanderplas, A. Passos, D. Cournapeau, M. Brucher, M. Perrot, and E. Duchesnay. Scikit-learn: Machine learning in Python. Journal of Machine Learning Research, 2011