

# LUKAS FESSER

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## EDUCATION

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### Harvard University

- PhD in Applied Mathematics.
- MSc in Computer Science.

2024-28

### University of Oxford

- MSc in Mathematics, *with Distinction*.

2021-22

### Yale-NUS College

- BSc in Mathematics and Computer Science, *Summa cum Laude*.

2017-21

## RESEARCH INTERESTS

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**Geometric Deep Learning:** Graph and topological neural networks, topology and geometry-based encodings, methods for understanding and improving generalization and extrapolation capabilities.

**AI for Healthcare:** LLMs for medicine, biomedical knowledge graphs, drug interaction prediction.

## EXPERIENCE

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### Avelios Medical, Munich, Germany

- Machine Learning Engineer.

06/2024 - 09/2024

- Developed ML-based workflow recommendation systems for clinical practitioners. Trained vision models on dermatological datasets for disease classification. Finetuned open-source LLMs on medical data to improve summarization and classification capabilities, particularly on non-English datasets.

### Harvard Department of Economics, Cambridge, MA.

- Pre-doctoral Fellow in Machine Learning

07/2022 - 06/2024

- Worked with Prof. Melissa Dell on deep learning models for economics, including vision, NLP, and graph-based models. Analyzed large economic datasets using network analysis and statistical modeling.

## TECHNICAL SKILLS

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**Programming Languages:** Python, C/ C++, R, Matlab, OCaml

**ML Libraries:** PyTorch, TensorFlow, Sklearn

**Other Software & Tools:** AWS, Microsoft Azure, CUDA, LaTeX, Git

## PUBLICATIONS & PAPERS UNDER REVIEW

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[9] **Performance Heterogeneity in Message-passing and Transformer-based Graph Neural Networks**

*Lukas Fesser and Melanie Weber. "Graph-level Heterogeneity in Message-passing and Transformer-based Graph Neural Networks", under Review at International Conference on Learning Representations (ICLR) 2025.*

[8] **Balancing Fairness and Accuracy in Graph Learning via Fairness-constrained Rewiring**

*Jason Wang\*, Lukas Fesser\*, and Melanie Weber. "Balancing Fairness and Accuracy in Graph Learning via Fairness-Constrained Rewiring", under Review at Learning on Graphs (LoG) 2024.*

[7] **Unitary Convolutions for Learning on Graphs and Groups**

*Bobak Kiani, Lukas Fesser, and Melanie Weber. "Unitary Convolutions for Learning on Graphs and Groups", Neural Information Processing Systems (NeurIPS) 2024. **Spotlight**. Arxiv version.*

[6] **Understanding and Mitigating Extrapolation Failures in Physics-informed Neural Networks**

**Lukas Fesser\***, Richard Qiu\*, and Luca D’Amico-Wong\*. “Understanding and Mitigating Extrapolation Failures in Physics-informed Neural Networks”, under Review. Arxiv version.

[5] **Scalable Polyhedral Robustness Verification for Scene-Text Recognition**

Daqian Shao, **Lukas Fesser**, and Marta Kwiatkowska. “Scalable Polyhedral Robustness Verification for Scene-Text Recognition”, under Review. Arxiv version.

[4] **Augmentations of Forman’s Ricci Curvature and their Applications in Community Detection**

**Lukas Fesser\***, Sergio Serrano\*, Karel Devriendt, Melanie Weber, and Renaud Lambiotte. “Augmentations of Forman’s Ricci Curvature and their Applications in Community Detection”, *Journal of Physics: Complexity*, 2024. Arxiv version.

[3] **Effective Structural Encodings via Local Curvature Profiles**

**Lukas Fesser** and Melanie Weber. “Effective Structural Encodings via Local Curvature Profiles”, *International Conference on Learning Representations (ICLR) 2024*. Arxiv version.

[2] **Mitigating Over-smoothing and Over-squashing using Augmentations of Forman-Ricci Curvature**

**Lukas Fesser** and Melanie Weber. “Mitigating Over-smoothing and Over-squashing using Augmentations of Forman-Ricci Curvature”, *Learning on Graphs (LOG) 2023*. Arxiv version.

[1] **Tightness of Bernoulli Gibbsian line ensembles**

Evgeni Dimitrov\*, Xiang Fang\*, **Lukas Fesser\***, Christian Serio\*, Carson Teitler\*, and Weitao Zhu\*. “Tightness of Bernoulli Gibbsian line ensembles”, *Electronic Journal of Probability* 2021. Journal version. Extended Arxiv version.

## SELECTED HONORS

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- Kempner Institute Graduate Fellowship	2024
- Trinity College Academic Excellence Award	2022
- Trinity College Graduate Fellowship	2021
- Yale-NUS Academic Merit Scholarship	2017

## ONGOING PROJECTS

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**On the Role of Initialization and Encodings in Attention-based Graph Neural Networks**  
with Bobak Kiani and Melanie Weber.

**Extrapolation and Generalization Capabilities in Knowledge Graph Foundation Models**  
with Marinka Zitnik.

**Structural and Positional Encodings for Hypergraph Neural Networks**  
with Raphael Pellegrin and Melanie Weber.

## LANGUAGE SKILLS

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<b>Fluent:</b>	German (native), English, French
<b>Conversational:</b>	Spanish, Mandarin Chinese