Jakub Vrábel

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Вю

I am a fifth-year Ph.D. candidate in applied physics. My specialization is in interpretable machine learning (ML) for spectroscopic data and physics-inspired learning. Recently, I have become interested in foundational ML, where I work on mode connectivity, sparsity (lottery tickets), and overparametrization (NTK, double descent). My goal is to contribute to interpretable and safe ML/AI.

Education

| 2019 - present | Ph.D. candidate in applied physics Central E | European Institute of Technology (CZ) |
|----------------|---|---------------------------------------|
| 2024 - present | visiting grad. student (superv. David Krueger) | University of Cambridge (UK) |
| 2021 - 2022 | visiting grad. student (superv. Hans Lohninger) | Technische Universität Wien (AT) |
| 2017 - 2019 | Master's deg appl. physics (with distinction) | FME, Brno University of Technology |
| 2016 - 2017 | additional Bc. studies - appl. physics | FME, Brno University of Technology |
| 2013 - 2016 | Bachelor's degree - mechatronics | FME, Brno University of Technology |
| extra courses: | statistical physics of fields, GTR, advanced quan | tum mech., Lie groups, data mining |

WORK EXPERIENCE

| 2016 - present | Research associate – CEITEC (CZ), Group of Laser Spectroscopy |
|----------------|---|
| | Topic: machine learning for spectroscopic data, laser-induced plasma physics |
| 2018 | Research intern – Complutense University of Madrid (ES), 6 months |
| | Topic: characterization of laser-induced plasmas (with prof. Caceres) |
| 2015 - 2017 | Multimedia specialist – Moravia IT (now RWS) (CZ), part-time |
| | Localization of Microsoft Office (video editing, vector/raster graphics, scripting) |

Summer schools

| 2023 | IAIFI Summer School - Physics and AI (Boston, USA) |
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| | ELLIS Summer School - Probabilistic ML (Cambridge, UK) |
| 2022 | IAIFI Summer School - Physics and AI (Boston, USA) |
| | Arnold Sommerfeld Centre Summer School - Physics meets AI (Munich, DE) |
| | Erwin Schrödinger Institute Summer School – ML for materials (Vienna, AT) |
| 2021 | Machine Learning in Quantum Physics and Chemistry Summer School (Warsaw, PL) |

Selected Publications

- 2023 Spectral library transfer between distinct Laser-Induced Breakdown Spectroscopy systems trained on simultaneous measurements. Vrábel, J. et al. JAAS, IF 4.35 DOI: 10.1039/D2JA00406B
- 2022 Improving laser-induced breakdown spectroscopy regression models via transfer learning. Képeš, E., **Vrábel, J.** et al. JAAS, IF 4.35 DOI: 10.1039/D2JA00180B
- 2021 Interpreting support vector machines applied in laser-induced breakdown spectroscopy. Képeš, E.,
 Vrábel, J. et al. Analytica Chim. Acta, IF 6.91 DOI: 10.1016/j.aca.2021.339352
- 2020 Restricted Boltzmann Machine method for dimensionality reduction of large spectroscopic data. Vrábel, J. et al. Spectrochim. Acta B, IF 3.66 DOI: 10.1016/j.sab.2020.105849
- 2020 Benchmark classification dataset for laser-induced breakdown spectroscopy. Képeš, E., Vrábel,
 J. et al. Scientific Data, IF 8.50 DOI: 10.1038/s41597-020-0396-8
- * a complete list of publications can be found on Google Scholar

- H-index: 9 (250 citations)
- 14 journal articles
- 7 conference talks, 4 posters

CONFERENCES

- 2024 Youth in High Dimensions (Trieste, IT) 2023 IAIFI workshop (Boston, USA) 2022 SCIX (Covington - KY, USA) 2022LEA (Tokyo, JP) 2022 IAIFI workshop (Boston, USA) LIBS2022 (Bari, IT) 2022 2021 EMSLIBS (Gijon, ES) 2020 LIBS2020 (Kyoto, JP) 2020 IOM-LIBS (fully-online) 2019 EMSLIBS (Brno, CZ) 2017 EMSLIBS (Pisa, IT)
- Skills

machine learning (artificial neural networks, kernel methods), statistical physics, Python (JAX, Pytorch, scikit-learn, Pandas), R (data processing, visualization), GitHub, cloud & GPU computing (Azure, GCP)

OTHER ACHIEVEMENTS & ACTIVITIES

Josef Hlávka award, 2nd place in the Competition of Young Spectroscopists (IMMSS), rector's honorable mention, involved in 3 national-wide and 2 international projects, teaching seminars for Physics 1& 2.

ONGOING WORK

- 1. *Input space mode connectivity* (with D. Krueger, University of Cambridge). (manuscript under preparation). We extend the concept of loss landscape mode connectivity to the input space of deep neural networks. We explore and show applications of the concept for interpretability and adversarial detection. My role: concept, numerical experiments, theory.
- 2. Sparse interpretable neural networks for spectroscopic data. (manuscript under preparation). I study various approaches to achieve sparse models that are natively interpretable. This includes L1 and custom-developed regularizations, and lottery tickets. My role: concept, numerical experiments, theory.
- 3. Neural tangent kernel (NTK) & double descent (with O. Shem-Ur and Y. Oz, Tel Aviv University). In this project, we aim to find connections between linearization (NTK regime) and overparametrization in neural networks. My role: numerical experiments.

FURTHER CAREER PLAN

With a deep passion for science, particularly physics and ML, I am driven to learn and explore these areas continuously. My aim is to make valuable contributions to the scientific community. My next objective is to find a postdoc or industry-research position that aligns with my interests and aspirations.

- PI of 5 student projects (funding $50,000 \in$)
- 3 book chapters (all published by Wiley)
- superv. of 5 students (bachelor, internship)

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