Jakub Vrábel

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Bio

I am a fourth-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 sparsity (lottery tickets), overparametrization (NTK, double descent, mode connectivity), and general interpretability.

Education

2019 - present	Ph.D. candidate - applied physics	Central European Institute of Technology (CZ)
2017 - 2019	Master's deg. - appl. physics (*with honors*)	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 quantum 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

2021 - 2022 — Research intern – TU Wien (AT), 3 months
Topic: topological data analysis for hyperspectral images (with prof. Lohninger)

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)

Stats

- H-index: 9 (250 citations)
- 14 journal articles
- 7 conference talks, 4 posters
- PI of 5 student projects (funding 50,000 €)
- 3 book chapters (all published by Wiley)
- superv. of 3 students (bachelor, internship)

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

Summer schools

2023	IAIFI Summer School - Physics and AI (Boston, USA)
	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)

Conferences

2023	IAIFI workshop (Boston, USA)	poster
2022	SCIX (Covington - KY, USA)	oral presentation
2022	LEA (Tokyo, JP)	(online) oral presentation
2022	IAIFI workshop (Boston, USA)	poster
2022	LIBS2022 (Bari, IT)	oral presentation
2021	EMSLIBS (Gijon, ES)	(online) oral presentation
2020	LIBS2020 (Kyoto, JP)	(online) oral presentation
2020	IOM-LIBS (fully-online)	(online) oral presentation
2019	EMSLIBS (Brno, CZ)	poster and oral presentation
2017	EMSLIBS (Pisa, IT)	poster

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, rector's honorable mention, involved in 3 national-wide projects, teaching seminars from Physics 1 and Physics 2 at FME Brno University of Technology

Ongoing Work

1. *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.
2. *Initialization of ANN weights with simulated spectra (in the first layer).* We aim to achieve better performance and interpretability by starting from a physics-relevant position in the parameter space (i.e. physics-informed learning). Initial values of weights can be handcrafted to contain inductive biases for specific tasks. My role: concept, numerical experiments.
3. *Neural tangent kernel (NTK) & double descent* (in collaboration with O. Shem-Ur, Tel Aviv University). In this project, we aim to find connections between linearization (NTK regime) and over-parametrization in neural networks. My role: numerical experiments.

Further career plan

With a deep passion for science, particularly in the field of physics and machine learning, I am driven to continuously learn and explore these areas. Supported by an international network of brilliant scientists and colleagues, 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.