ODYSSEAS VAVOURAKIS

DPhil (PhD) Student, University of Oxford — ML for Biomolecular Structure

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EDUCATION

DPhil (PhD) - Department of Statistics
University of Oxford (Balliol College), UK

📅 Sep 2023 – present

- focus on **ML for Protein Design** (SABS:R^3 CDT)
- first-year student, currently pursuing rotation projects
- coursework in software engineering, mathematical modelling, structural drug discovery, data science, and scientific computing

M.Sc. Computational Biology & Bioinformatics
ETH Zürich, Switzerland

📅 Sep 2020 – Aug 2023

- graduated **with distinction**; **ranked 1st** in my course
- **top grade for thesis project** (see right-hand column)
- **GPA: 5.9 / 6.0** ($= \mu + 1.75\sigma$); UK 1st class equivalent
- totalled **151 / 120 ECTS credits**; extra coursework in RL & probabilistic ML, NLP, computational quantum chemistry and physics, game theory
- jointly awarded with Universities of Zurich and Basel

B.Sc. Biochemistry
Heidelberg University, Germany

📅 Sep 2015 – Aug 2018

- **GPA 1.5** (best possible: 1.0)
- extra coursework on computational methods

PUBLICATIONS

Exact tunneling splittings from symmetrized path integrals
G. Trenins, L. Meuser, H. Bertschi, O. Vavourakis, R. Flütsch, and J. O. Richardson

📅 2023   📍 Journal of Chemical Physics

- https://doi.org/10.1063/5.0158879
- a new path-integral molecular dynamics simulation technique to calculate exact ground-state tunnelling splitting patterns in small molecules without wavefunctions

INTERESTS

Geometric DL   Generative Models
Comp. Protein Design   Biomolecular ML
Comp. Biophys.   Bayesian ML   Phylogenetic Inference
Evolutionary & Learning Dynamics   Physical Chemistry

RESEARCH EXPERIENCE

Rotation Project
De Novo **Generative Antibody Design**

📅 Mar 2024-present   📍 OPIG, University of Oxford

- *in silico* antibody design with generative AI
- advised by Prof C. Deane; Dr F. Dreyer & Dr D. Cutting

Master's Thesis Project
Boost-SE: Wide-Spectrum Enzyme-Substrate Interactions from Multi-Task Recommendations using Protein Language Models

📅 7 months (2023)   📍 ETH AI Center, ETH Zürich

- recommendation system to propose likely-interacting enzyme-substrate pairs given a set of MACCS fingerprints + enzyme sequences
- enables inductive enzyme and compound discovery
- trained on binary, positive/unlabelled metabolic pathway data + auxiliary targets
- uses fine-tuned pLM sequence embeddings
- advised by Prof A. Krause, J. Rothfuss, M. Mutný

Rotation Project
Calculating Tunnelling Splittings with Path-Integral Molecular Dynamics

📅 3.5 months (2022)   📍 D-CHAB, ETH Zurich

- helped develop the mathematical method, implemented and validated the sampling scheme and estimator
- built path-integral molecular dynamics simulation package from scratch
- see publication on left
- advised by Prof J. Richardson; Dr G. Trenins

Bachelor's Thesis Project
Spectrin-Repeat Mechanical Unfolding with Atomistic Force-Probe MD

📅 3.5 months (2018)   📍 HITS, Heidelberg

- studied rupture force and sequence determinants of unfolding behaviour of spectrin repeat domains under mechanical tension with force-probe molecular dynamics (GROMACS)
- advised by Prof F. Gräter; Dr C. Daday

SKILLS

Python & PyTorch
R
C++
Other
Git, Shell & UNIX, Docker, LaTeX

DISTINCTIONS

Willi Studer Prize 2024, as top graduate of the year in my degree course at ETH Zürich.
📅 2024

Oxford University **Clarendon Scholar**
Oxford University **Scatcherd European Scholar**
Balliol College **John Henry Jones Scholar**
📅 2023-2028

Scholar at **Studienstiftung des deutschen Volkes** (German Academic Scholarship Foundation)
📅 2015-2018 and 2020-2023 (B.Sc. and M.Sc.)

WORK EXPERIENCE

Sergeant (NATO OR-5; Military Service)
Hellenic Air Force
📅 Nov 2018 - Nov 2019   📍 Athens, Greece

- **Clinical Biochem – General Air Force Hospital**
  - photometric/spectroscopic sample analysis, clinical assessment and reporting; responsible for ER samples; technical maintenance
- **Fuel Chemist – Eleusis Air Base**
  - scanning electron microscopy of engine micro-debris for predictive maintenance
  - aircraft fuel and engine lubricant quality control and contamination assessment (i.a. optical emission spectroscopy)

LABORATORY EXPERIENCE

Degree-Associated Practicals
### Heidelberg University
📅 2015 - 2017   📍 Heidelberg, Germany

- **Biochemistry:** experience in lipidomics; lipid click chemistry; FACS; CRISPR knockouts; immunoprecipitation (ChIP/qPCR); HPTLC; fluorescence microscopy; retroviral transduction; cloning; protein interaction & kinetic assays; protein purification; primer design
- **(In)Organic Chemistry:** AAS, IR, Raman, EI MS, 1D & 2D NMR; small molecule crystallography & theory; multi-stage organic and inorganic synthesis; classical quantitative analysis (potentiometry, conductometry, electrogravimetry etc.);
  non-spectroscopic inorganic analysis

LANGUAGES

Language	Level
English	●●●●●
German	●●●●●
Modern Greek	●●●●●
Spanish	●●●○○
Latin	●◐○○○
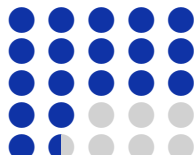
CO-CURRICULARS

Cooperativeness in Graph-Based Systems
Summer Game Theory Course Project
📅 Summer 2021   📍 ETH Zurich

- studied collective phase changes in cooperative behaviour in agents facing iterated prisoner's dilemma interactions while interconnected in a dynamic random graph structure
- three-person group project; won best presentation

Information Theory & Evolution
Summer School/Academic Retreat
📅 Summer 2016   📍 Ftan, Switzerland

- two-week workshop on information-theoretic approaches to the evolution of intelligence
- gave introductory presentation on information theory
- co-wrote agent-based simulation framework to model emergence of intelligence (three-person group project)

LEISURE

- online lectures/courses
- seminar talks, podcasts, non-fiction reading
- language learning, linguistics