

Andrea Karlová

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University College London, London, United Kingdom
Department of Computer Science, 2015 - present
Research Student

- collaboration with University of Surrey ([Prof. Ravi Silva](#)) and UCL AI Centre ([Prof. Brooks Paige](#)) on high-throughput system for various perovskites photovoltaics discovery
used methods: evaluation of the atomic structures using various quantum mechanical computations to determine the bandgap ([GPAW](#) and [ASE](#) packages, [RDKit](#), pymatgen, psi4, pySCF, Material Project), various geometric deep learning methods (Graph Neural Networks with Message Passing, DNNs for Surfaces), SMILES compressing VAEs, material science pretrained word embeddings
- robustness of latent representations
used methods: Optimal Transport Theory, VAEs, GECO for fine-tuning beta-VAEs
MSc thesis co-supervised at UCL CS:
 - Cen, Huisan, *On the Topic of Density Functional Theory with Deep Learning*, September 2021
 - Ortega Gonzales, Alvaro, *Enhancing Variational Monte Carlo with SVGD and Kernel Herding*, September 2021
 - Penciu, Andrei, GENTRL, September 2021
- collaboration with University of Chemistry and Technology, Prague, Czech Republic ([Prof. Daniel Svozil](#)) on virtual screening for drug-discovery
used methods: VAEs applied to molecular fingerprints (ECFP and FCFP) producing chemically semantic latents, RL for molecular design generation, docking

Education

Pursuing PhD in Computer Science, University College London, United Kingdom	present
Pursued PhD in Mathematics, Charles University, Prague, Czech Republic (PhD title not gained in 2013 due to death of supervisor)	2014
Mgr. (BS + MSc) in Mathematics, Charles University, Prague, Czech Republic	2005

Employment

Tech & Startups: 2017 - present

April19 Discovery Ltd., June 2021 - present

ML R&D Consultancy

- Molecular Drug Design for drugs penetrating central nervous system
used methods: similarity searching, QSAR models and multi-task DNNs for target-assay pair prediction, bioactivity prediction, generative models in drug discovery

Fractal Labs Ltd., July 2018 – August 2020

Senior Data Scientist, Data Science Lead

- Time-series forecasting for Small and Medium Enterprises cash flow
used methods: VAEs applied to time series, time warping loss function, Neural ODEs, various CNNs and RNNs based architectures, Random Forests, Kalman Filters
- Domain Specific Conversational chatbot for Small and Medium Enterprises
used methods: various CNNs and RNNs based architectures for Language Understanding Unit (NER model, Intent Classifier), Q-learning with memory reply (Dialog Manager component), VAEs

(Language Generation)

- full production pipeline for ML models: Tensorflow Extended, docker
- worked on R&D grant applications: awarded 300k GBP InnovateUK grant (Project Lead)
- active collaboration with University of Bristol and UCL CS on MSc. student projects supervision

MSc thesis co-supervised:

Stein, Adam, *Neural Variational Inference for Text Generation*, May 2019

Pabrinkis, Aurimas, *Measuring the Spatial Distortions Caused by Embeddings*, September 2019

StatusToday, November 2017 – April 2018

Data Science and R&D

- created and developed employee productivity analytics based on user file activity recognition
used methods: randomised intensities of Compound Poisson processes and change points detection

Academic and Research Positions: 2010 - 2016

University College London, London, United Kingdom

Department of Computer Science, 2015

Visiting Research Student

- preliminary research into constructing financial instruments based on intellectual property and related trading platform
used methods: hidden Markov models, market making strategies using RL
- calibration of tempered Levy Flights volatility surfaces to the FX market data
- supervision of MSc student final theses:
Munir, Necati, *Creating a Trading Platform for Intellectual Property Trading*, April 2016.
Zhao, Yaolin, *Trading Simulation in the Intellectual Property Market*, September 2015.

University College London, London, United Kingdom

Department of Civil, Environmental & Geomatic Engineering, 2015

Developer

- testing scalability of a high-volume Fusion and Analysis platform for geospatial clouds which was co-funded by European Commission (FP7 2002 – 2013, [IQmulus project](#))

Gorilla Science, 2011 - 2016

PhD and research funding

- long running collaboration with [Dr. Patrick S. Hagan](#) on the term structure volatility surface models using tempered Levy Flights in order to produce robust hedges for forward starting products
results first presented at: RISK Event Quant Summit 2016 Europe, April 2016
used methods: partial integral differential equations, stochastic calculus for pure jump processes, perturbation theory, complex variables

Imperial College London, Department of Mathematics, 2015-2016

Visiting Research Student

- fixed income models driven by tempered Levy Flights

University of Oxford, The Oxford-Man Institute of Quantitative Finance, 2010

Visiting Research Student

- computational methods for option pricing models driven by stable laws
results presented at: QMF Quantitative Methods in Finance, Sydney, 2010

Columbia University, Department of Statistics, 2010

Visiting Research Student

- developing numerical solutions for option pricing models driven by stable laws
results presented at: seminar talk at Rutgers University

Financial Industry: 2005 - 2010

PricewaterhouseCoopers Czech Republic, 2009 - 2011

Consultant

- pricing exotic financial derivatives and illiquid products

KBC Global Services, Group Value and Risk Management, 2006 – 2008

Model Validation, Associate

- validation of Interest Rate Derivatives and Life Insurance Derivatives models

CSOB (member of KBC Group), Risk Management Department, 2005 - 2009

Market Risk, Associate

- market risk methodology, independent price verification, reporting to the Board of Executives
- quantitative researcher for commodity trading models

Selected Publications

1. (2021) Karlová A., Dehaen W., Penciu A.; [How to Reward Your Drug Agent](#), December 2021, Conference Workshop: DGMs and Applications NeurIPS 2021
2. (2021) Karlová A., Underwood C., Silva R.; [Virtual Screening For Perovskites Discovery](#), July 2021, Workshop: Tackling Climate Change with ML, ICML 2021
3. (2021) Karlová A., Dehaen W., Svozil D.; [Molecular Fingerprint VAE](#), July 2021, Conference Workshop: WCB ICML 2021
4. (2020) Karlová A.; [Robustness of Latent Representations](#), July 2020, Conference Workshop Proceedings UDL ICML 2020
5. (2018) Klebanov L., Karlová A.; [Distributional Tail Estimation through its Characteristic Function](#), Mar 2018, Journal of Mathematical Sciences, Vol. 229, Issue 6, pp 714–718
6. (2016) Karlová A., Hagan P.S.; [On Beyond Black](#); Sept. 2016, Wilmott, p.42-69
7. (2013) Karlová A.; [On distribution of product of stable laws](#); SIAM Theory of Probability and its Applications (submitted September 2013, accepted July 2015)
8. (2008) A. Karlová; *Levy Processes and Balayage Spaces*; J. Antoch., G. Dohnal, (Eds.) ROBUST 2008, Proceedings of the 13th Summer School of the Union of Czech Mathematicians and Physicists, 171—176.

Selected Talks

1. [AI UK, London](#) 2021
2. QuantInsights, London 2019
3. Women in Data Science, 2019, Tel Aviv, 2019
4. [49th London PyData Meetup](#) 2018
5. RISK Event Quant Summit 2016 Europe 2016
6. Quantitative Methods in Finance, QMF 2010, Sydney, Australia 2010

Programming Skills and Languages:

- programming languages: Python, C/C++, Bash
- libraries: Python – Tensorflow, SciPy, Numpy, Pandas, ScikitLearn
- other tools: SQL, MongoDB, git, docker, AWS
- operating system: Linux (Debian)

Grants, Honours, Awards:

[Best Poster Award WCB ICML 2021](#), [InnovateUK \(2019\)](#), [Bio-Math Summer School and Workshop. Middelfart, Denmark \(2008\)](#), 'Stochastic Differential Equation Models with Applications to the Insulin-Glucose System and Neuronal Modelling' at Satellite Summer School on Levy Processes, funded under

Marie Curie EU grant contract. Sandbjerg, Denmark (2007), 'Statistics for stochastic differential equations models' at EMS Summer School, Séminaire Européen de Statistique, funded under Marie Curie EU grant contract. Cartagena, Spain (2007), Global Association of Risk Professionals Seminar under scholarship from Agence de Transfert de Technologie Financiere. Luxembourg (2005)