

# 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 pre-trained 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
- 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
- UCL CS MSc student projects supervision:
  - Penciu, Andrei, *Generative Modelling for Drug Design*, September 2021

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. [49<sup>th</sup> 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)