

1 Contact details

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2 Summary

I enjoy problem solving and coming up with creative solutions. I am a proficient programmer in both C and Python and also have familiarity with Matlab and Fortran. I am also familiar with the OpenCV library for computer vision and have used Tensorflow and Keras extensively throughout my PhD.

2.1 PhD thesis summary

My PhD research, conducted under the supervision of Dr Richard Bryce and Dr Neil Burton, focused on the use of machine learning to make force predictions with applications to molecular dynamics simulations. During the course of the research a multitude of novel artificial neural network architectures were designed and implemented using the Tensorflow library. Additionally a scheme was created allowing chemically intuitive pairwise forces to be calculated from total Cartesian forces. The created machine learned force field was then utilized within a molecular dynamics code I wrote in order to run simulations of small drug like molecules, including aspirin.

3 Skills

- Experience with neural networks and their applications to a wide range of problems.
- Experience with the Tensorflow library.
- An understanding of a wide range of machine learning techniques and their applications.
- Proficiency in C and Python.
- Experience with Matlab and Fortran.
- A reasonable understanding of geometry optimization techniques, with a focus on Molecular Dynamics.
- A reasonable understanding of computer vision techniques and their applications.

4 Work History

4.1 Order Management – 07/2013 to 09/2013

Percy Group – Altrincham

- Creation of custom scripts to speed up processing orders.
- Creation of a bar-coding system to ensure accuracy when dispatching orders.
- Use of specialist order management software such as Linnworks and Magento.
- Research into the profitability of different product lines and providing advice based on this.

4.2 Assistant – 08/2018 to 09/2018

The University of Manchester – Manchester

Creation of new lab script, spreadsheets for data processing, test questions as well as health and safety work, for first year labs.

4.3 Teaching assistant – 2019 to 2020

Annually taught a 4 week course on modelling the growth of zeolite crystals by writing custom Fortran scripts. Also helped with the Matlab course and an introduction to visualizing proteins course.

5 Education

5.1 Undergraduate - University of Manchester

Mchem 2:1

- 3rd year project focused on the use of computer vision to track the propagation of chemical waves produced by the Belousov–Zhabotinsky reaction in a petri dish.
- 4th year project was the use of neural networks to speed up powder averaging for EPR calculations.

5.2 Postgraduate

PhD, thesis title ‘Quantum mechanical methods for in silico drug design: Force predictions via machine learning with applications to molecular dynamics simulations’

6 Extra curricular and accomplishments

- Was a member of the Member of Unmanned Aerial Vehicles (UAV) society.
- Developed for and attended the international micro air vehicle conference and competition (IMAV) 2014, achieved 7th place internationally in the competition.
- Chief scouts gold award.
- International Chemistry Olympiad – Bronze award
- Cambridge Chemistry Challenge – Copper award
- University of Manchester 3 minute thesis competition - first place
- Department of Pharmacy and Optometry showcase second place for the speaking competition, later served as a judge for the competition.
- Thales arduino contest - first place at Manchester University.