# PENELOPE JONES

Gonville and Caius College, Trinity Street, Cambridge, CB2 1TA (+44) 788 940 3321  $\diamond$  pj321@cam.ac.uk

# **EDUCATION**

# Gonville and Caius College, University of Cambridge

2019 - Present

Ph.D. Physics

Supervisor: Dr Alpha Lee

Areas of Study: Machine learning, Bayesian inference, and their application in drug discovery and smart

charging of energy storage devices.

# Pembroke College, University of Cambridge

2015 - 2019

M.Sci. Experimental and Theoretical Physics

B.A. NATURAL SCIENCES

Research Project: 'Automated discovery of physics from molecular simulations using machine 83.0% learning' (supervised by Dr Alpha Lee).

EnterpriseTech: Investigation into the potential of a research project to be translated into marketable technology (Judge Business School).

| Part III: Class I | 77.6% |
|-------------------|-------|
| Part II: Class I  | 79.3% |
| Part IB: Class I  | 81.0% |
| Part IA: Class I  | 83.6% |

#### RESEARCH

# Bayesian inference reveals hidden structure in concentrated electrolytes

Electrostatic correlations between ions in concentrated electrolytes are not well understood, despite being of crucial importance in a huge range of applications, from self assembly of biopolymers to energy storage in supercapacitors. I used Bayesian unsupervised learning to infer the number of statistically distinct local environments, and their characteristics, within such systems. *Under review*.

# Determining an optimal supercapacitor charging strategy using Bayesian optimisation

Counter-intuitively, it has been observed in simulations that continuous application of the maximum voltage does not attain maximal supercapacitor charging over a given time period. The question arises: can we determine the optimal charging strategy? We use Bayesian optimisation to find such a strategy, collecting both real and simulation experimental data. Working paper.

## Biochemical data imputation with reliable uncertainty estimates

Most biochemical databases are sparsely populated, and many compounds are discounted in the early stages of the drug discovery process due to this lack of experimental data. Accurate imputation of missing values, with good uncertainty estimates, would dramatically increase the compound search space. I use a deep neural network and a training procedure inspired by that used for training neural processes to attain state-of-the-art performance on multiple biochemical datasets. Working paper.

## ACADEMIC AWARDS AND PUBLICATIONS

## ICLR Workshop on Fundamental Science in the Era of AI

2020

Poster titled 'Benchmarking scalable active learning strategies on molecules'.

# Oppenheimer Studentship

2019 - Present

Winton Scholarship

2019 - Present

# Gordon Research Conference on Chemistry and Physics of Liquids

2019

Poster titled 'Deciphering the structure of concentrated electrolytes using unsupervised learning'.

# Foundation Scholarship, Pembroke College

2017, 2018, 2019

For performance in the Natural Sciences Tripos.

**BP Prize** 2016

For outstanding performance in Part IA Chemistry (2<sup>nd</sup> out of 600 students).

Dr Stevens Prize 2016

For performance in Part IA Natural Sciences (7<sup>th</sup> out of 600 students).

College Scholarship, Pembroke College 2016

For performance in Part IA Natural Sciences.

**British Chemistry Olympiad** 2015

Top 50 in the UK.

**British Physics Olympiad** 2015

Top 100 in the UK.

British Physics Olympiad Experimental Prize 2014

For producing the best A-level project in the UK.

## WORK EXPERIENCE

#### JP Morgan Cazenove 2017

Investment Banking Summer Analyst

# The Cambridge Union

2016 - 2018

Treasurer

I initiated and organised several large debates on topics including artificial intelligence and driverless cars. I competed alongside and against industry experts on behalf of the Cambridge Union in its inaugural debate abroad, in Paris, on the topic of artificial intelligence.

#### **TEACHING**

# Undergraduate Supervisor, University of Cambridge

2019 - Present

I supervise Part IA Natural Sciences undergraduates in the Mathematics A and Mathematics B modules.

# Private Tutor, Pembroke Tutors

2017 - 2020

I tutored GCSE and A-level students in preparation for their Mathematics and Physics examinations.

## TECHNICAL STRENGTHS

**Machine Learning Frameworks** PyTorch, scikit-learn

**Programming Languages** 

Python

# REFEREES

Available on request.