Sam Ireland, PhD

A freelance software developer, highly proficient in web development, Python, Javascript and machine learning.

Deep Mountain

Contracting (2020-)

I operate as a freelance developer, primarily in the bioinformatics and drug development space. I have completed several fixed term projects since starting operations last year.

Goodwright

Director (2019-)

A software company I run with a friend. We make web-based software primarily for academia, as well as custom applications for clients' requirements.

University College London

PhD Student (2016-2021)

Thesis: Predicting and Characterising Zinc Binding in Structure and Sequence

Centre for Integrative Physiology

Research Fellow/Developer (2015-2016)

A one year project to create a database of druggable protein components from the existing Guide to Pharmacology.

University of Edinburgh

Undergraduate (2011-2015)

Grade: First Class Hons.

Dissertation: Investigating the effects of using Semi-empirical Quantum Mechanical Methods to improve Structure-based Virtual Screening

Positions: Section Editor of *The Student*

Rossall School

Secondary School (2002-2009)

International Baccalaureate (42/45 points)

Python

Eleven years of experience, and strong familiarity with the vast majority of both Python and Pythonic principles. I am the author of the Python library atomium, and various smaller libraries.

Django

Six years of experience, and used in almost all web projects I have undertaken in that time. Familiar with middleware, the Django ORM and its optimisations, the Django template system, and Gunicorn. My Django projects include standalone template-based sites, as well as backends for REST and GraphQL APIs.

Javascript

Sixteen years of experience, with particularly heavy use in the past four years. I am familiar with most ES6+ features, and am comfortable with Promises, async/await, both ES6 and node modules, NPM, and Javascript's various idiosyncracies.

React

Extensive experience over multiple projects over the past three years. I am familiar with both class-based and functional/hooks-based components, (with a preference for the latter) and typically use the Apollo Client library for communicating with GraphQL backends.

GraphQL

I have created multiple applications using GraphQL (including two of the first ever publicly available bioinformatics APIs over GraphQL - ZincBindDB and ZincBindPredict), am the author of the Python GraphQL client kirjava, and am in the process of writing a review of the uses of graphQL in bioinformatics. I am convinced of GraphQL's advantages over REST, and have pivoted my projects accordingly in recent times.

Machine Learning

A good understanding of the major concepts of machine learning, both deep and otherwise, and experience in creating supervised learning systems from scratch.

Test Driven Development

I am both a proponent and strict user of unit and functional tests, viewing them as a key component of writing code from the ground up, rather than an addendum at the end of development. I also maintain comprehensive documentation for most of my widely used libraries, and adopt a documentation-first approach when coding.

Server/Container Management

I am comfortable on the backend of applications, being primarily responsible for the servers of our Goodwright applications, and my own projects. Familiar with Linux (mostly Ubuntu/CentOS), PostgreSQL, gunicorn, Docker, and Bash. I use DigitalOcean and AWS for VPSs.

Bioinformatics

I have spent the last six years in various Bioinformatics roles, and am particularly adept at structural bioinformatics. Creating the Python atomium library has given me a very detailed knowlwedge of the PDB, CIF and MMTF file formats, as well as the various computational manipulations of protein structures.

Publications

Zincbindpredict—Prediction of Zinc Binding Sites in Proteins
2021 Molecules

atomium - a Python structure parser
2020 Bioinformatics

ZincBind - The Database of Zinc Binding Sites
2019 Database

Inverse pharmacology: Approaches and tools for introducing druggability into engineered proteins
2019 Biotechnology Advances

SynPharm: A Guide to PHARMACOLOGY Database Tool for Designing Drug Control into Engineered Proteins
2018 ACS Omega

The IUPHAR/BPS Guide to PHARMACOLOGY in 2018: updates and expansion to encompass the new guide to IMMUNOPHARMACOLOGY
2017 Nucleic Acids Research

Thermal melt circular dichroism spectroscopic studies for identifying stabilising amphipathic molecules for the voltage-gated sodium channel NavMs
2017 Biopolymers

Projects

atomium
atomium.samireland.com

A python library for parsing protein structures in .pdb, .cif, or.mmtf format, building them into biological assemblies, and analysing them. This is my most widely used library, most developed library (over 1,200 commits) as well as the library with the most comprehensive test suite.

ZincBind
zincbind.net

The database of zinc binding sites, built for my PhD. A bioinformatics pipeline constructs the database from the Protein Data Bank entries and a set of Random Forest models use this data to create predictive models of zinc binding for both structure and sequence.

pdb2json
pdb2json.samireland.com

A lightweight API wrapper around atomium for representing any PDB structure as JSON. This is a very minmal, single-file django app.

election19
election19.samireland.com

A visualisation of the 2019 UK election, as well as an interface for modelling the outcome if voting patterns had been different in user-defined ways. This was a weekend analytics project.

samireland.com
samireland.com

My personal portfolio website, built with Django. It showcases the projects I work on, as well as serving as a place to publish articles.

lytiko
lytiko.com

A personal analytics and quantified-self platform, which is built using React, Django, and GraphQL. This is currently my main hobby project.

kirjava
kirjava.samireland.com

A Python library for creating GraphQL queries in an easy-to-use, Pythonic way. Initially an exercise in learning how GraphQL schemas worked, it is now used in production in various other projects of mine.

Goodwright Projects

These are public-facing projects carried out as part of Goodwright, which I co-run. Broadly speaking, I am responsible for the backend and Javascript in these projects.

LabTab
labtab.io

A lab management tool for lab PIs, built with React, Django, and GraphQL. This project has very much been a UI/UX-first design, with minute details honed for ease of use for the end user.

iMaps
imaps.goodwright.org

A bioinformatics analysis tool for RNA-protein binding data. This React/GraphQL application allows users to perform analysis pipelines on their data without using the terminal.

Various Lab Websites

We have created various lab websites showcasing research, to the specifications of the PI involved. This has been invaluable in honing the art of working to a client's requirements. Examples include branco-lab.org, rochefortlab.co.uk, jyxborderconsulting.co.uk and hebenstreitlab.org.

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