Abstract

Open Python Workshop Series 1 (Monday, 16 Nov 2020) – Tracing the Covid-19 Curve - Uplifting Your Data Visualization Skills with Python

You have probably seen enough Covid-19 curves that trace daily cases country-by-country. Some of these looks amazingly good, and some even offer interactive tools for you to explore the data. Given that there are 195 countries in the world and we are nearly a year into the pandemic, there is already a lot of data!

How can people make the tracing curve so informative? How can I attempt one to visualize my research data? In this virtual tutorial, we will show you how to make one with Python by covering a few basics:

- Jupyter notebook
- Basic data handling with Python programming
- Plotting static data with Matplotlib, and quick tricks to make your graphs instantly look better!
- Bringing interactive tools with Bokeh package, and finally
- Machine-Learnings – How can you start with just less than ten lines of code!

Open Python Workshop Series 2 (Monday, 30 Nov 2020) – Machine Learning 101 Using Python

The subject matter to be covered in this session will provide opportunities to build upon the data visualization skills acquired from the previous event and help you develop a visual understanding on what machine learning (ML) is really trying to do ‘behind-the-scenes’.

Jack will use simple examples to demonstrate key concepts and model training procedures for supervised ML, a technique used to surrogate a quantitative relationship from the observed data.

During this live event, Jack will not only be teaching how to fit a curve, but also provide an opportunity to learn some other very interesting aspects of ML.
Open Python Workshop Series 3 (Monday, 14 Dec 2020) – **Pattern Discovery with Unsupervised Machine Learning**

In the second workshop Jack will discuss the fundamental principles of supervised machine learnings with simple, visualisable examples. In this workshop, Jack will cover another important category of machine learning, namely, the unsupervised machine learning.

We live in a complex world and most of the data gathered is multi-dimensional. While we are all capable of visualising trends and discovering patterns in a three-dimensional world, we generally do quite poorly when trying to comprehend complexities beyond that. Unsupervised machine learning can help us to discover intriguing relationships within the data, as well as building sensible two-dimensional projections in order to visualise these relationships. In the past it was not referred to as “machine learning” but it was, and still is, widely used across many different fields.

Similar to the previous Python workshops, we will be using simple and visualisable data to demonstrate how it works and Jack will address other cross-cutting aspects of machine learnings that were not discussed in the previous workshop.

**I have no prior coding experiences or I just don't like programming...** Don't worry, all you need is a bit of curiosity. Jack used to swear to himself that he will NEVER EVER program again after he did a C course in computational physics as an undergrad. As you can tell, that never happened. It's much easier these days with Python!

**Biography**

Dr Jack Yang is currently a Lecturer in the Materials and Manufacturing Futures Institute and School of Material Science and Engineering at UNSW. He received his BSc in Nanotech in 2007 and PhD in 2011, from the same institute. Before returning to UNSW in 2017, he was a Postdoctoral Fellow in world-leading research groups of computational chemistry, first at Organic Chemistry Institute of Westfälische Wilhelms-Universität Münster from 2011 to 2013, Germany and then in the School of Chemistry at University of Southampton, United Kingdom from 2013 to 2017. During his time in Southampton, he participated in the sixth world-wide organic crystal structure prediction blind test (0.7M CPU hours), which he and his team were amongst top three performing groups, out of total 25.

His current research focuses on applying global structure optimizations, quantum simulations and machine-learning techniques to explore the energy-structure-functional relationships in complex materials, including organic semiconductor crystals and multifunctional perovskites. Jack is also an active developer for research software in computational chemistry that harness the power of modern HPC facilities to perform high-throughput screenings of functional materials.

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**Registration Link:** [https://ntu-sg.zoom.us/meeting/register/tJcuc-6tgzMpGNFHGGvP6PmxnvmN5_77zbte](https://ntu-sg.zoom.us/meeting/register/tJcuc-6tgzMpGNFHGGvP6PmxnvmN5_77zbte)

**Hosted by:** Associate Professor Ng Kee Woei