Machine Learning for Chemists

Some useful information to go with the course "Machine Learning for Chemists"

Course contact

If you have any questions regarding the content of the course please feel free to drop me an email at k.butler@reading.ac.uk or keith.butler@stfc.ac.uk

Interactive notebooks

The course includes interactive notebooks and these will be used for the practical and the assessment. All notebooks can be run through *Google Colab*. You can find the notebooks here: https://github.com/keeeto/reading-ml-chemistry

The instructions to run the notebooks in *Colab* are at that location also. If you find that you lose the notebooks at any time, just return to this page and you can reload them following the instructions.

Saving notebooks

- If you want to save and reload the notebooks you will need to save a copy of the original notebook to your *Google Drive*
- Go to File > Save copy in Drive
- When you want to reload navigate to: http://colab.research.google.com/
- Got to File > Open
- Choose the *Google Drive* tab, you should now see your saved notebooks.

Additional reading/resources

For an excellent no-nonsense overview I highly recommend the following blog post, it covers most of what we will do and some extra: https://vas3k.com/blog/machine_learning/

There is a book "Deep Learning for the Life Sciences" available in the University library. Although the course is not based on this book it does contain some useful information, particularly on deep neural networks. I would recommend Chapter 2, Chapter 4 and Chapter 11 in particular.

How decision trees work, YouTube: https://www.youtube.com/watch?v=DCZ3tsQIoGU&feature=youtu.be
Neural networks from the ground up, YouTube: https://www.youtube.com/watch?v=aircAruvnKk