## CoCalc (Collaborative Calculation; free plan): <a href="https://cocalc.com/">https://cocalc.com/</a>

- 1. Software compatibility
  - a. with GitHub: incompatibile (couldn't run notebooks directly from GitHub, or import a single notebook from GitHub)
  - b. Other sources
- 2. User friendliness:
  - a. Configurations / traffic: 1-core shared CPU
    - i. 1000MB of shared RAM
    - ii. 3000MB of disk space (per project).
    - iii. Sessions will shut down after 30 minutes of inactivity, though they can run for up to 24 hours.
  - b. Packages (<a href="https://cocalc.com/doc/software.html">https://cocalc.com/doc/software.html</a>)
    - i. additional packages: by request (not available for free plan)
    - ii. pre-installed for Python: https://cocalc.com/doc/software-python.html
  - c. Real-time collaboration: Yes
  - d. Shareable: Yes
  - e. Keep as a private file: Yes
  - f. Internet access: not available for a free plan
  - g. Shortcuts: 95% similar to Jupyter
  - h. **Version Control**: provides version control, "time travel", with excellent functionality
- 3. **Supporting languages (JupyterNotebook)**: using Linux terminal, CoCalc supports softwares including Bash, C++, C++ 17, GP, Haskell, JavaScript, Octave, Prolog, Python 2&3, R, Sagemath, Singular, Sparql
- 4. Customizability (&ease) of the configuration file:
  - a. .ipynb
  - b. .txt
  - c. .html
  - d. .md
  - e. .rst
  - f. .tex
  - g. .pdf
  - h. .sagews
  - i. .asciidoc
- 5. Speed of deployment (descriptions from the official website): "It takes less time to run a Jupyter Notebook than grabbing a cup of coffee!" (Zero setup, web-browser based)
- 6. Configurations

- a. Python Environments
  - i. already installed: <a href="https://cocalc.com/doc/software-python.html">https://cocalc.com/doc/software-python.html</a>
  - ii. request to install (only available for paid users):

    <a href="https://doc.cocalc.com/howto/install-python-lib.html">https://doc.cocalc.com/howto/install-python-lib.html</a> ###

ML-predict-drugclass-master It is impossible to run the provided JupyterNotebook under the free plan, since half of the libraries are not installed. Installing those libraries requires membership and installation requests.

- b. ML-predict-drugclass-master
  - i. Able to import:
    - 1. import os
    - 2. import random
    - 3. import time
    - 4. import warnings
    - 5. import numpy as np
    - 6. import pandas as pd
    - 7. import matplotlib.pyplot as plt
    - 8. **from pprint import** pprint
    - 9. **from collections import** Counter
    - 10. **from concurrent import** futures
    - 11. from IPython.core.display import Image
    - 12. from sklearn import preprocessing
    - 13. from sklearn.ensemble import RandomForestClassifier
    - 14. from sklearn.model selection import train test split
    - 15. from sklearn import metrics
    - 16. from sklearn.metrics import balanced accuracy score
    - 17. **from sklearn.metrics import** plot\_confusion\_matrix
  - ii. Need to request to install: rdkit, py3Dmol, mordred
    - 1. import py3Dmol
    - 2. **from mordred import** Calculator, descriptors
    - 3. **from rdkit import** DataStructs
    - 4. **from rdkit import** Chem
    - from rdkit.Chem import AllChem, Draw, rdDepictor, PandasTools
    - 6. from rdkit.Chem.Draw import IPythonConsole
    - from rdkit.Chem.Draw.MolDrawing import MolDrawing, DrawingOptions
- c. ML-TC1-master (Due to the limited capacity of RAM (1000 MB) and high requirements of CNN, the kernel crashed while running cell 19.)

- i. All libraries are able to be imported
- 7. Publications related to CoCalc
  - a. The CoCalc Wiki Pages (GitHub): <a href="https://github.com/sagemathinc/cocalc/wiki">https://github.com/sagemathinc/cocalc/wiki</a>
  - b Official
    - i. User Manual: <a href="https://doc.cocalc.com/contents.html">https://doc.cocalc.com/contents.html</a>
    - ii. Instructor guide: <a href="https://doc.cocalc.com/teaching-instructors.html">https://doc.cocalc.com/teaching-instructors.html</a>
    - iii. Student guide: <a href="https://doc.cocalc.com/teaching-students.html">https://doc.cocalc.com/teaching-students.html</a>
- 8. How effective is it to use these cloud deployments for running a workshop/teaching? <a href="https://doc.cocalc.com/teaching-instructors.html">https://doc.cocalc.com/teaching-instructors.html</a>
  - a. **Managed platform:** no time is wasted setting up, maintaining, backing up and securing a flaky platform. Instead, you can sleep while CoCalc ensures everything runs smoothly 24/7.
  - b. **Focus on helping students:** Jump right into a student's file and assist via a chat on the side
  - c. **Proven track record:** CoCalc has been used for teaching since 2013 in hundreds of courses by tens of thousands of students.
  - d. **Open source:** CoCalc itself and every software it offers is open-source. Say good-bye to vendor lock-in, hidden licensing fees, and proprietary black boxes.
  - e. Student work is isolated: Each student does course work in a separate project.

## 9. Summary

- a. Overall, I do not think CoCalc is an efficient and effective tool for teaching a Machine Learning workshop with following reasons:
  - i. Installing packages requires membership and is time-consuming.
  - ii. CoCalc has relatively smaller shared RAM and Storage, running complex models (such as Convolutional neural network) will results in a killed kernel
- b. Nevertheless, teaching more basic knowledge of Python is practical, with following available packages:
  - i. Python: https://cocalc.com/doc/software-python.html
  - ii. R: <a href="https://cocalc.com/doc/software-r.html">https://cocalc.com/doc/software-r.html</a>