Software Environment Setup

Machine Learning in Water and Environmental Modeling Pre-Workshop Setup Meeting, May 1, 2025

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Part A: Local Computer

Prerequisites

- Laptop or Desktop with Windows*
- 6GB free space
- Administrative privileges

^{*} The ML code will also run on Mac OS, Linux, and Google Colab

Overview

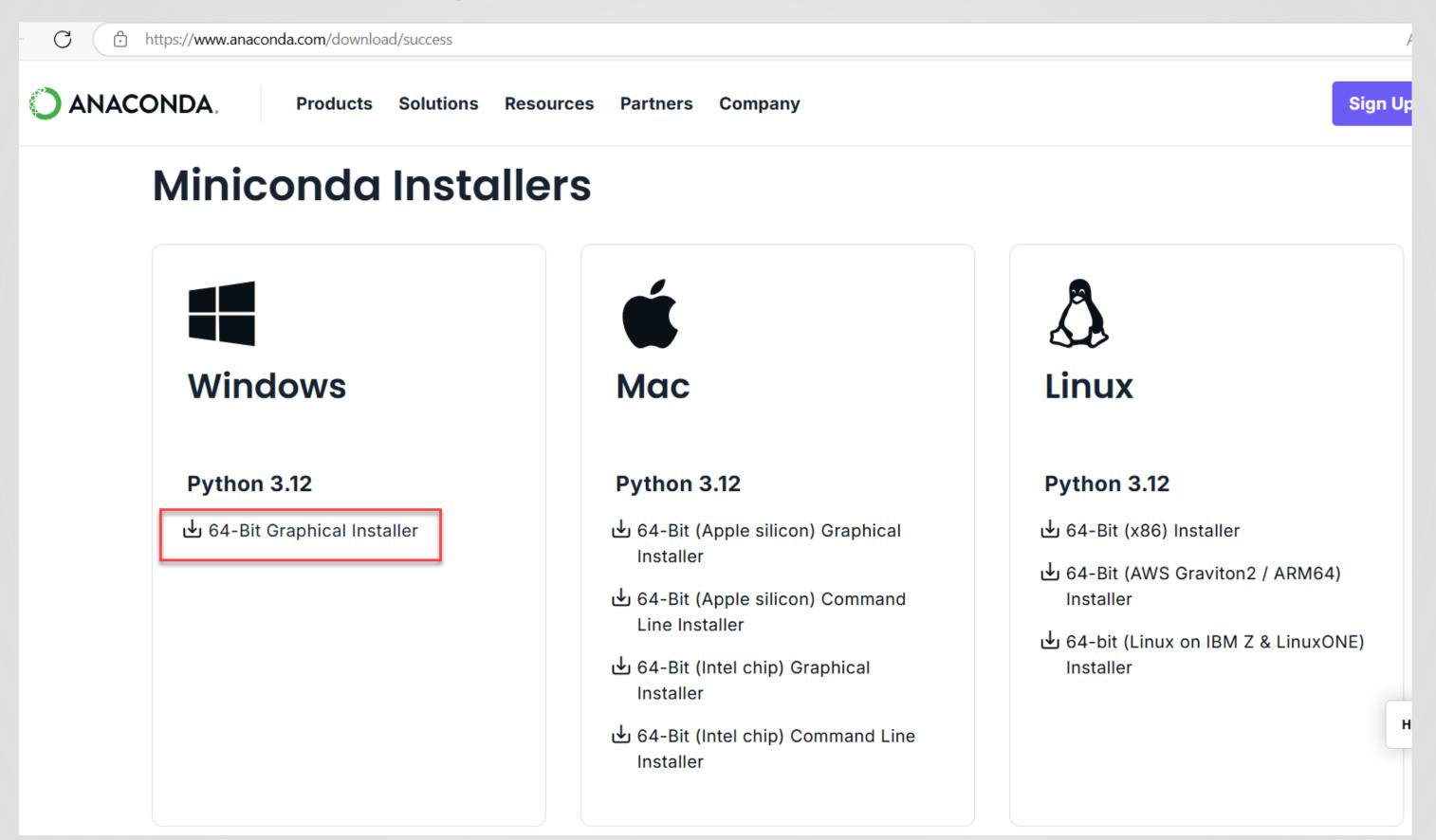
- Install Miniconda¹
- Create a conda environment²
- Download ANN code and input data files
- Run the Jupyter Notebook³ ANN code
- 1. Anaconda is a free, open-source platform that allows you to write and execute code in the Python programming language. Miniconda is a lightweight version of Anaconda. We recommend Miniconda because installation and setup take less time.
- 2. A conda environment is a folder containing a version of Python, and a specific set of python packages
- 3. Jupyter Notebook is a web application for creating and sharing computational documents

Install Miniconda/Anaconda

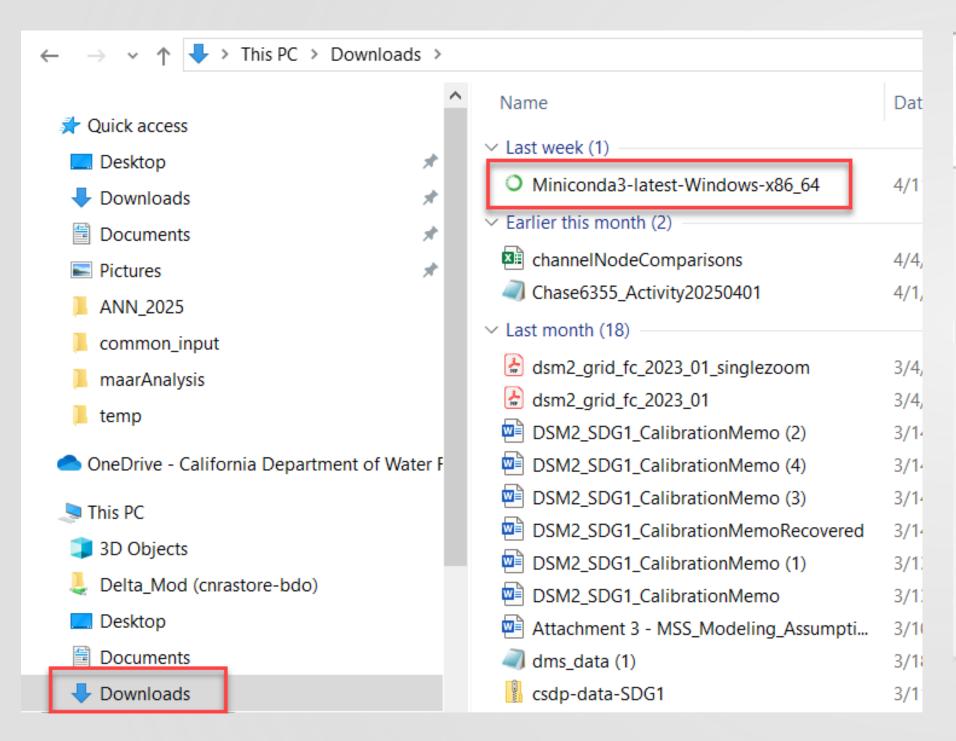
Miniconda or Anaconda:

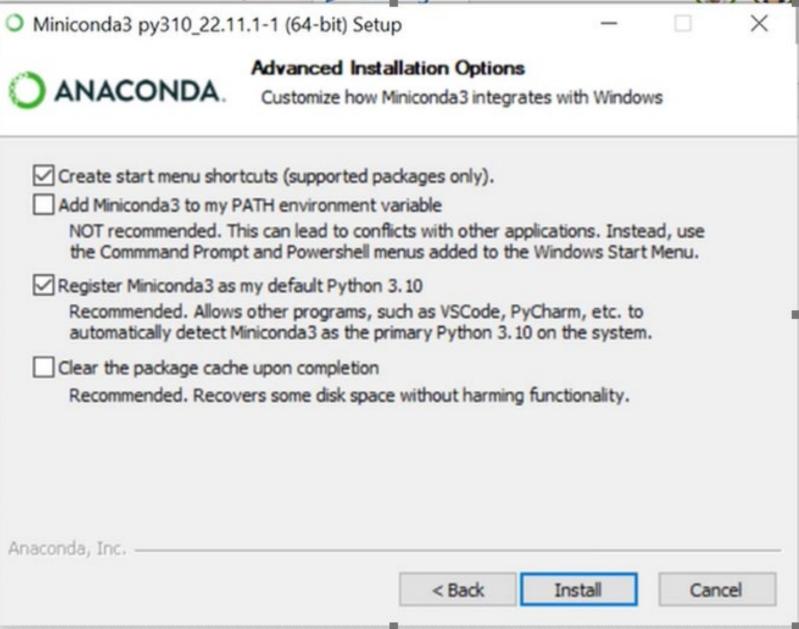
https://www.anaconda.com/download/success

Downloading the Miniconda Installer



Install Miniconda



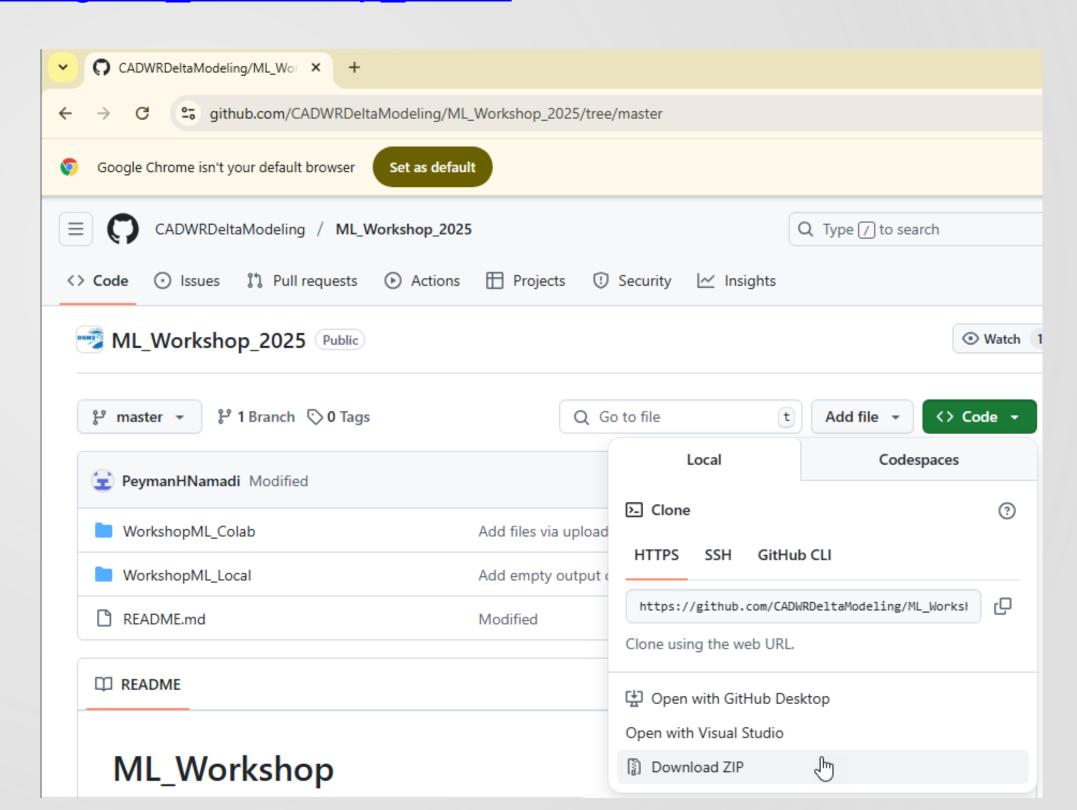


Download ML Code/Data

- a) If you don't have Git* installed
- https://github.com/CADWRDeltaModeling/ML Workshop 2025/

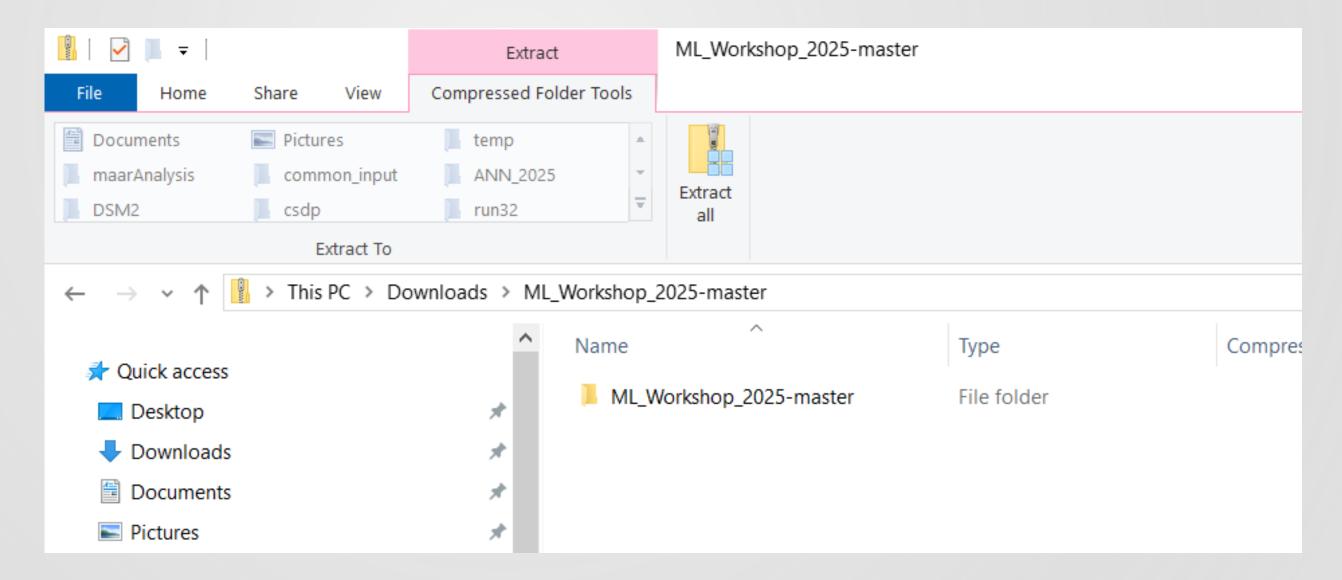
Click "Code", then "Download ZIP"

Git* is a free and open source distributed version control system

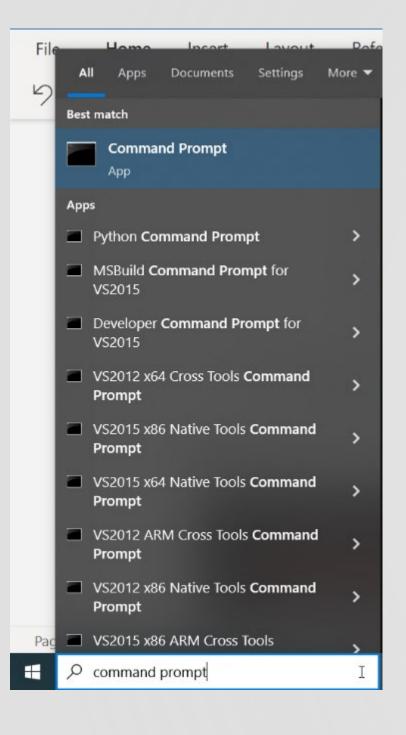


Download ML Code/Data

- a) If you don't have Git installed (cont)
- Double click the zip file
- Copy and paste the folder inside to another location



Download ML Code/Data



b) If you have Git installed
Open a command prompt window
Navigate to the location where you want to save files

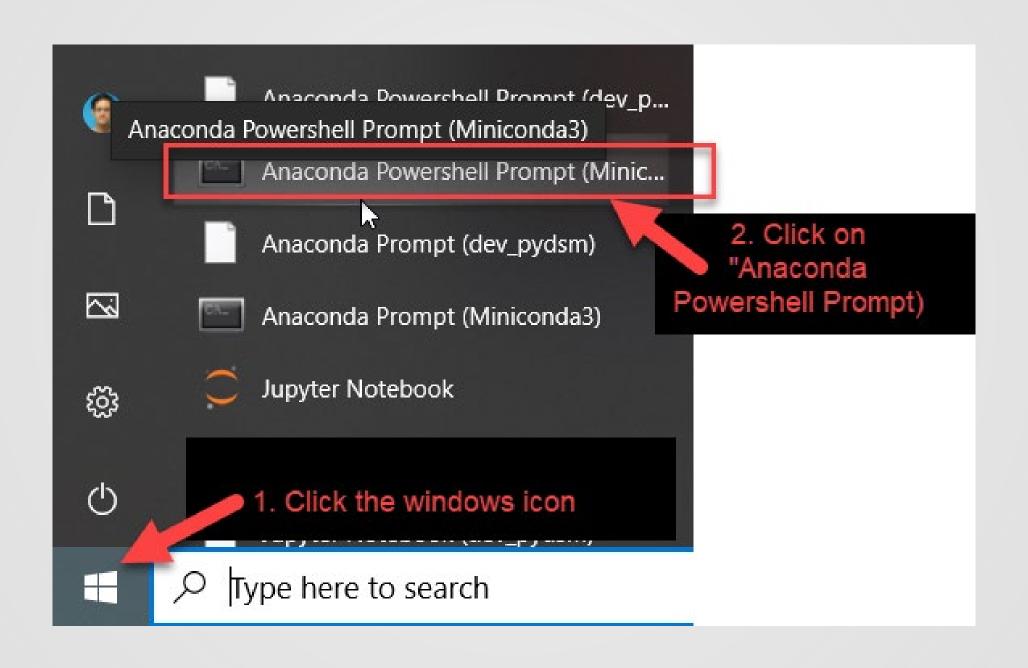
```
Select Anaconda Prompt (miniconda3)

(base) D:\temp>git clone https://github.com/CADWRDeltaModeling/ML_Workshop_2025
Cloning into 'ML_Workshop_2025'...
remote: Enumerating objects: 51, done.
remote: Counting objects: 100% (51/51), done.
remote: Compressing objects: 100% (28/28), done.
remote: Total 51 (delta 20), reused 51 (delta 20), pack-reused 0 (from 0)
Receiving objects: 100% (51/51), 1.73 MiB | 19.91 MiB/s, done.
Resolving deltas: 100% (20/20), done.

(base) D:\temp>_
```

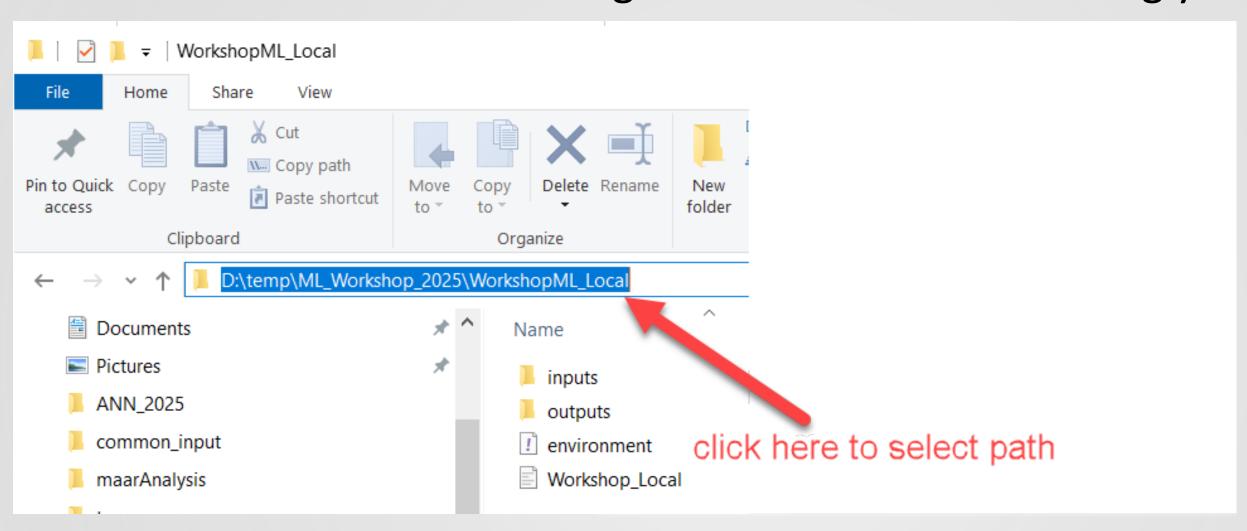
git clone https://github.com/CADWRDeltaModeling/ML_Workshop_2025

Open an Anaconda Powershell prompt



Create a conda environment

Use the "cd" command to navigate to the folder containing your code/data



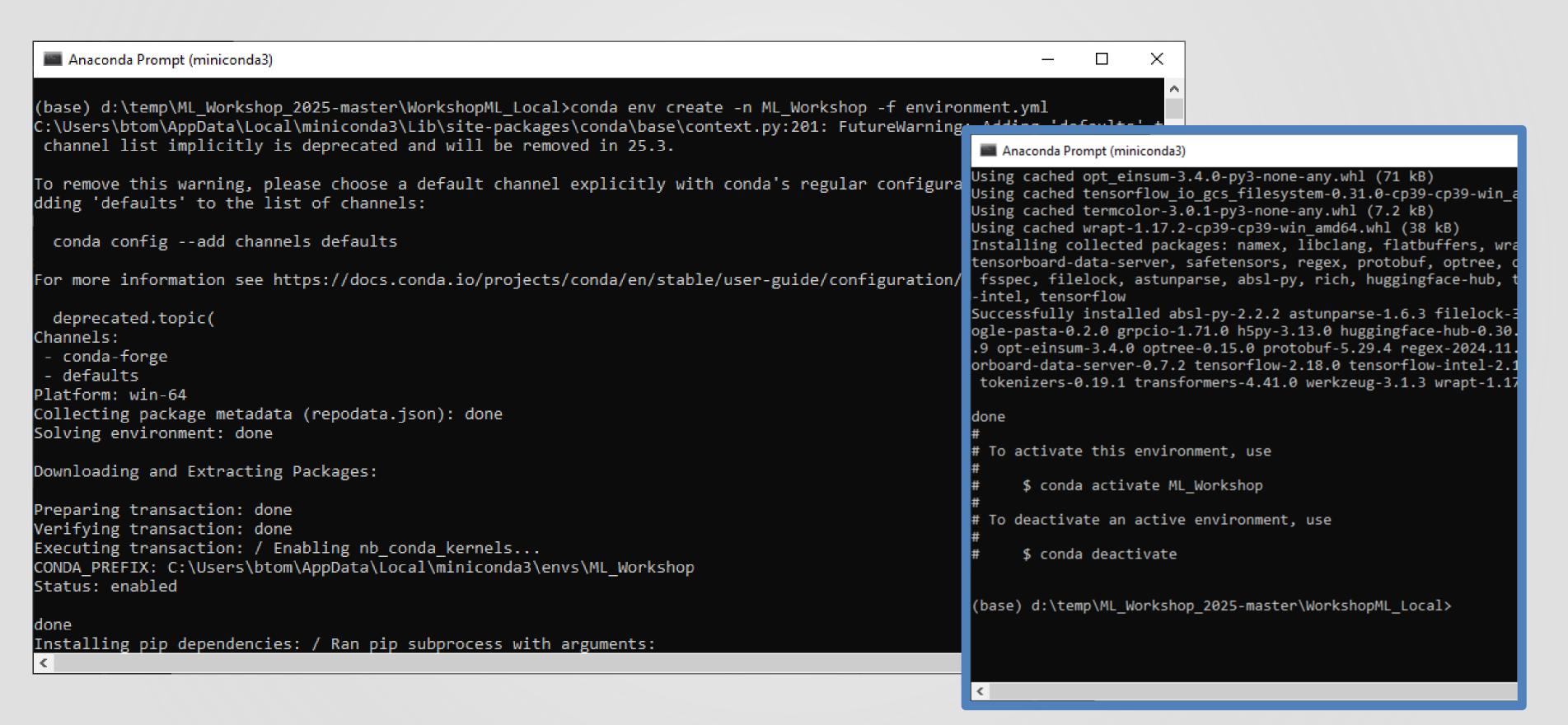
```
Anaconda Prompt (miniconda3)

(base) D:\temp>cd d:\temp\ML_Workshop_2025-master\WorkshopML_Local

(base) d:\temp\ML_Workshop_2025-master\WorkshopML_Local>_
```

Create a conda environment

conda env create -n ML_Workshop -f environment.yml



Open Jupyter Notebook

conda activate ML_Workshop jupyter notebook

```
Anaconda Prompt (miniconda3) - jupyter notebook

(base) d:\temp\ML_Workshop_2025-master\WorkshopML_Local>conda activate ML_Workshop

(ML_Workshop) d:\temp\ML_Workshop_2025-master\WorkshopML_Local>jupyter notebook

[I_2025-04-22_15:06:35.954_ServerApp] Extension package jupyter_lsp took 0.1534s to import

[I_2025-04-22_15:06:36.169_ServerApp] Extension package jupyter_server_terminals took 0.2141s to import
```

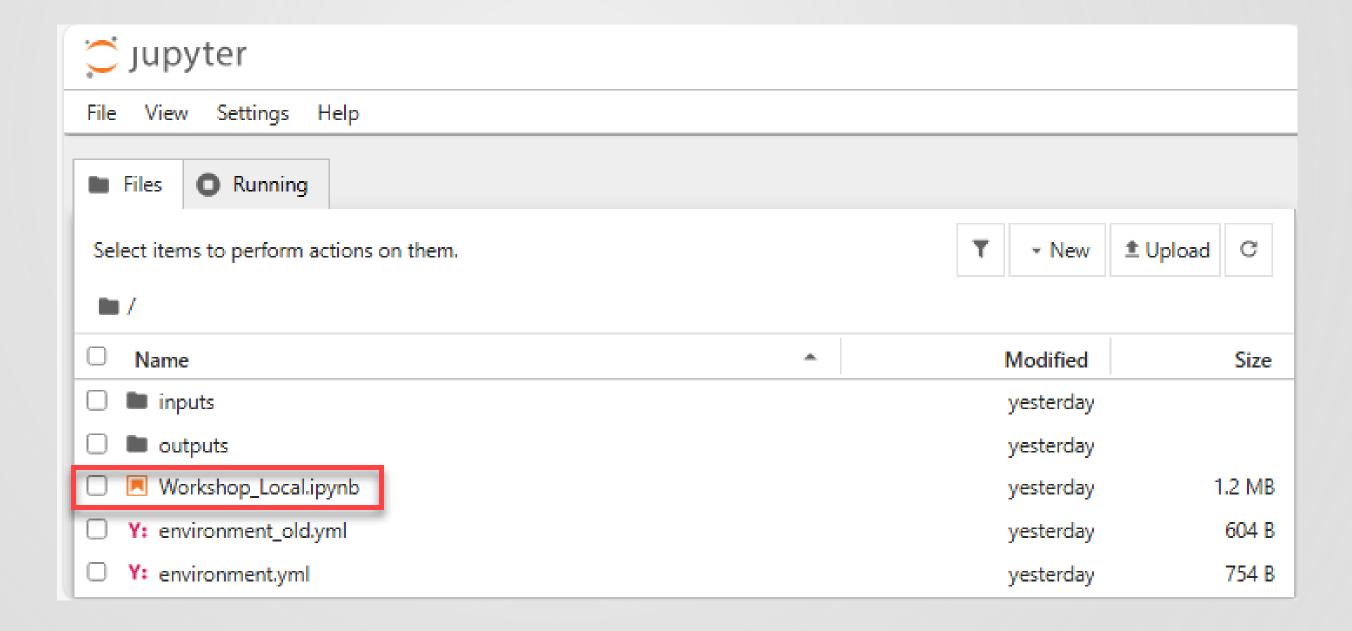
If the above command fails, try these two commands:

call conda activate jupyter start jupyter notebook

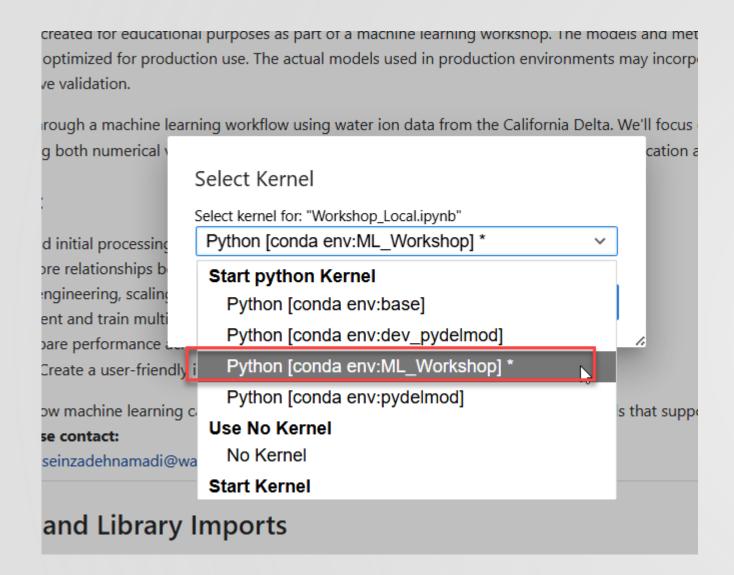
Open the ANN Jupyter Notebook

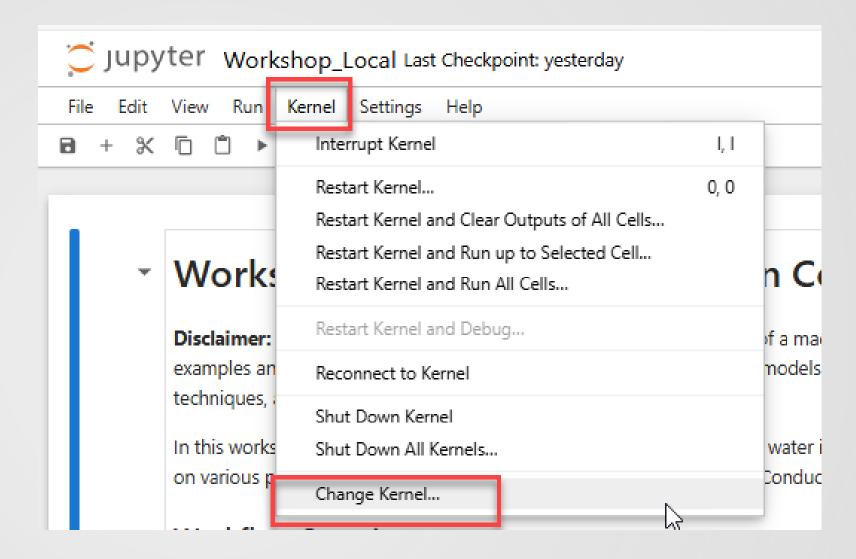
click on

Workshop_Local.ipynb

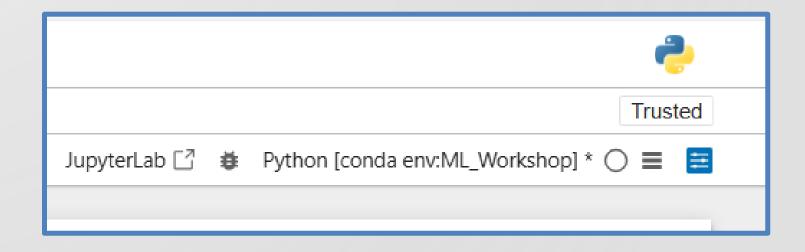


Select notebook kernel

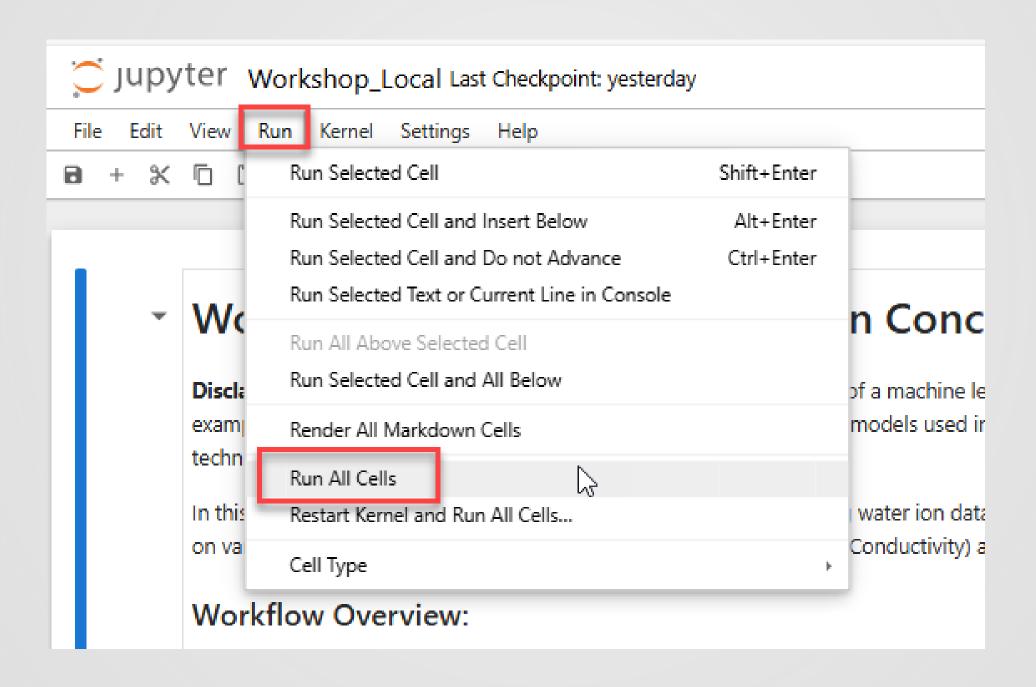




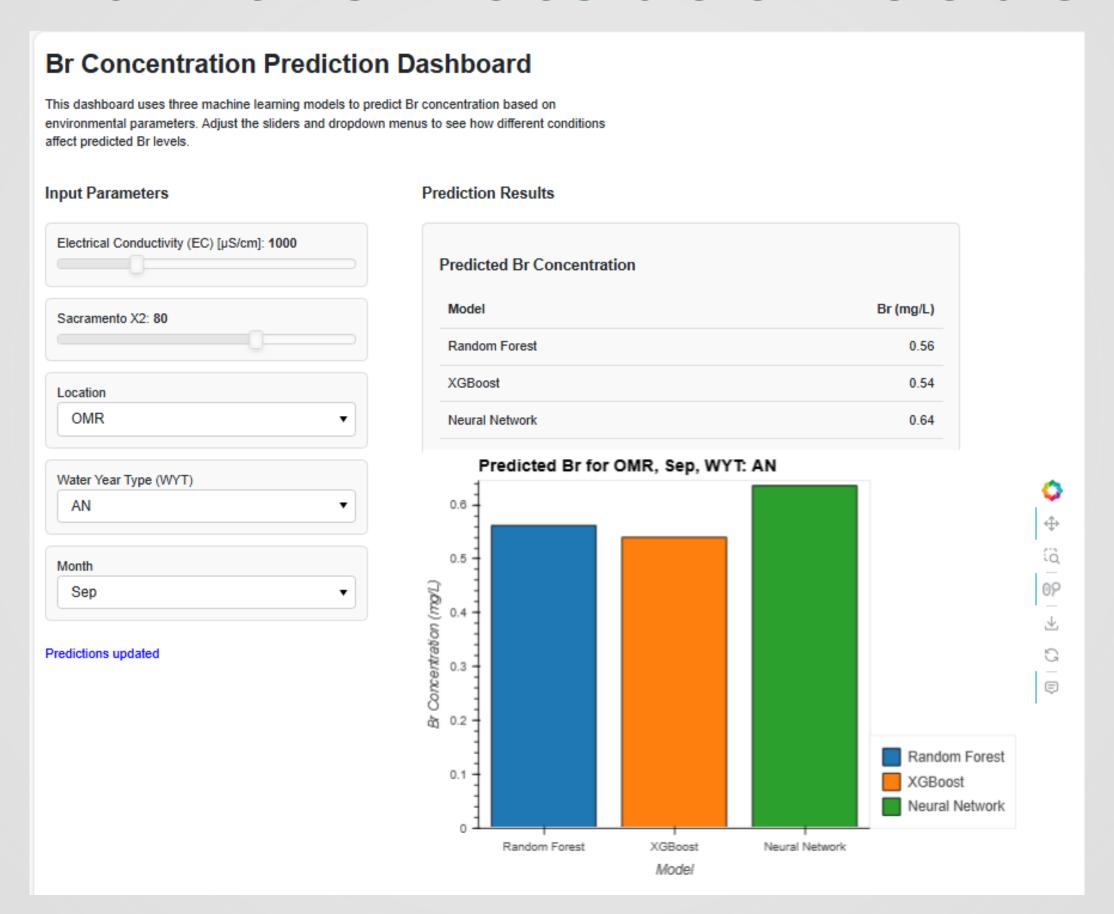
A notebook kernel is **a** "computational engine" that executes the code contained in a Notebook document.



Run the notebook code



Run the notebook code



Completed cell vs running cell

Section 0: Setup and Library Imports

1. Data Loading

```
[*]: import pandas as pd
import os

# Define the path to the inputs folder
input_folder = 'inputs'

# List of ion files to load
```

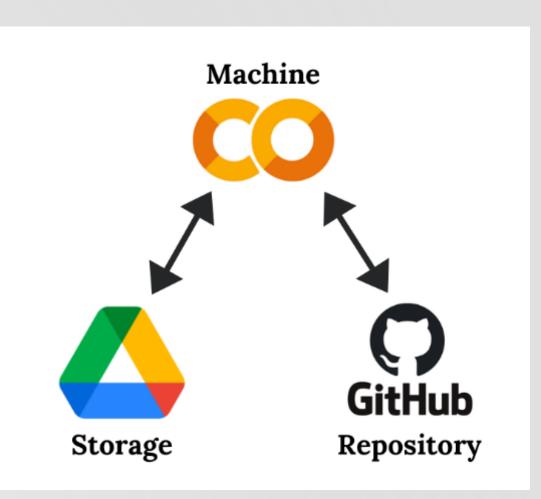
Part B:



Advantages of Google Colab:

- Free GPU/TPU access (to a certain limit)
- No setup required on your computer
- Real-time collaboration





Limitations of Google Colab:

- ➤ **Session time limits**: Free → 12-hour maximum runtime; paid tiers → 24 hours
- > Limited persistent storage: Files not saved to Google Drive are deleted when sessions end
- > Inconsistent performance: GPU/TPU availability and performance vary based on usage demand
- > Resource constraints: Limited RAM (typically 12-25GB) & storage capacity, especially on free tier



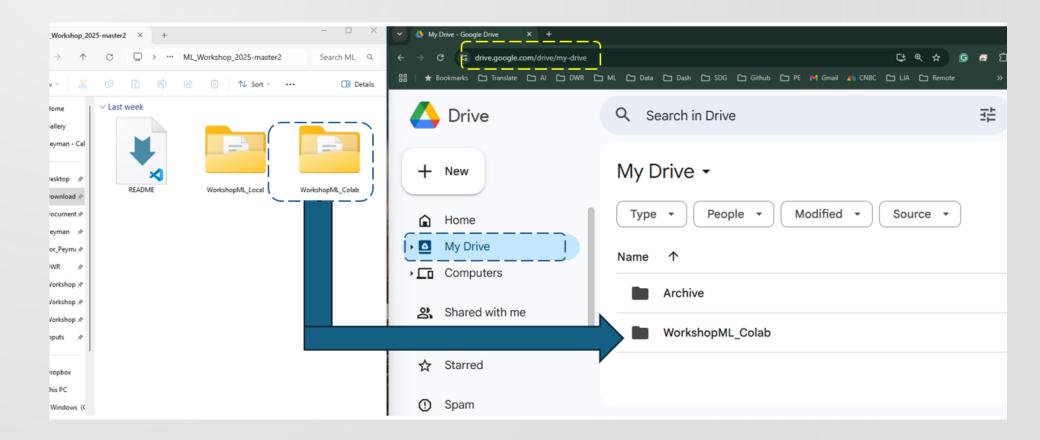
Step 1: Create a Google account or use an existing Google account and log in to your Google Drive at https://drive.google.com/drive/my-drive

Step 2: Use this link to download the folder containing data and code: https://github.com/CADWRDeltaModeling/ML Workshop 2025/tree/master

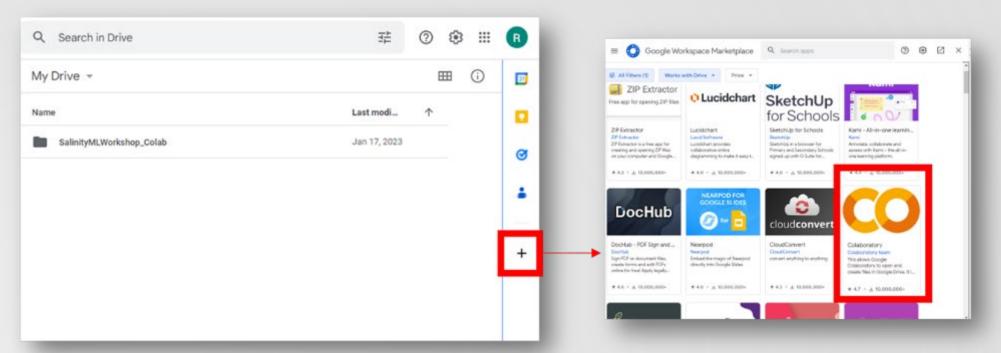


Step 3: Navigate to your download location and unzip the folder

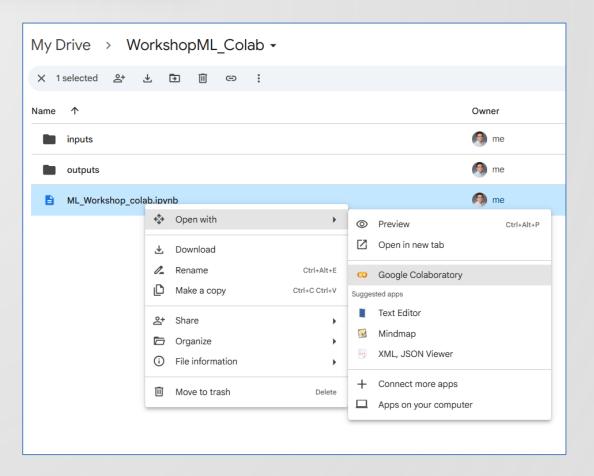
Step 4: After unzipping the file, you'll see two folders: "WorkshopML_Local" and "WorkshopML_Colab". Take the "WorkshopML_Colab" folder and upload it directly to the main area of your Google Drive (the "My Drive" section). Make sure you're uploading the actual folder with the workshop materials, not a parent folder that contains another folder with the same name.



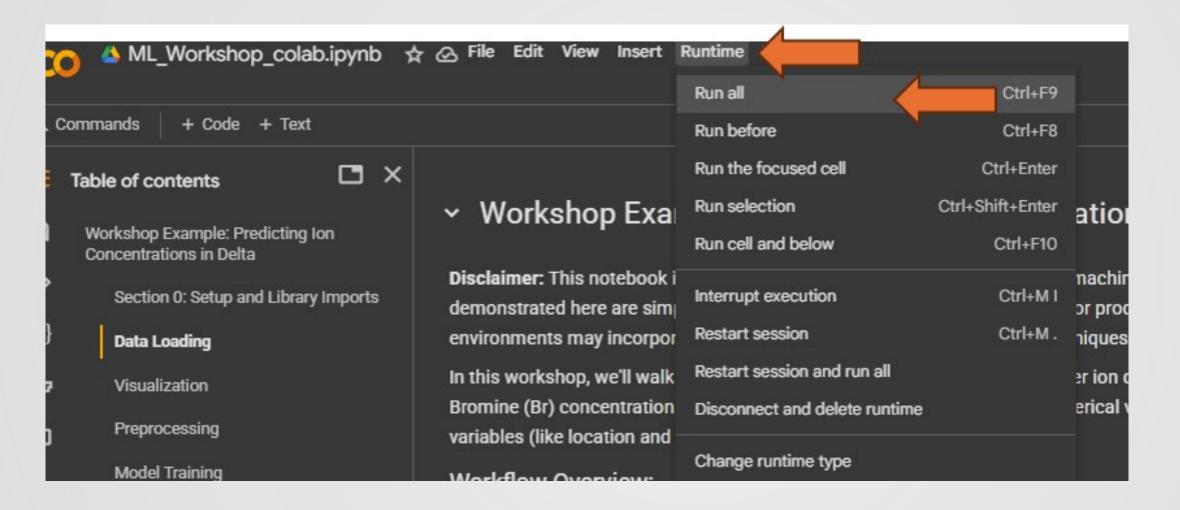
Step 5: Link the **Google Colab** Add-On to your Google Drive. See screenshot below. When complete, refresh your browser for the changes to take effect.



Step 6: Go into the "WorkshopML_Colab" folder you uploaded and open *ML_Workshop_colab.ipynb*. Right-click and Open With the Google Colaboratory.



Step 7: With the script now open in Colab, run the script by clicking *Runtime* and *Run All*. The script takes about 2 minutes to complete. Note: upon launching the code, Google Colab will request permission to access the folder – follow the prompts to allow access.



Questions?

