# 0. Setting Up – Installing Anaconda

## Python (<https://python.org/>) is a popular language for scientific computing, and great for general-purpose programming as well. Installing all of its scientific packages individually can be a bit difficult, however, so we recommend the all-in-one installer Anaconda. (5-10 min)

### Open the next link and downland the Anaconda Installer. Choose an installer compatible with your computer’s operating system.

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

Interfaz de usuario gráfica, Aplicación

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### Execute the anaconda installation file and complete the installation, keeping most of the default options.

1. Setting Up – Jupyter Notebook

## **Jupyter Notebook** is a web-based tool for creating and sharing documents with **live code**, **visualizations**, and **narrative text**. It's widely used in data science and machine learning for running code in blocks, viewing results instantly, and documenting the workflow, all in one place. Though it supports multiple languages, **Python** is the most common. (2 min)

### Search and run Anaconda Navigator in the Windows Start.

Captura de pantalla de un celular

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### In the Anaconda Navigator as shown below, click the Notebook’s Install button complete the installation.

Interfaz de usuario gráfica

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1. Virtual Environment Configuration

## Pyhton’s virtual environment is a tool that creates an independent space to manage projects and its modules and versions. In other words, it creates various workspaces on one serve/computer.

## Create a New Conda Environment (named cheminf) (2 min)

### Run **Anaconda Prompt** from Windows’s start menu. If you don’t see **Anaconda Prompt** installed, installed it using the Anaconda Navigator (previous point).

### Copy and paste this in your Prompt and press enter.

conda create -n cheminf python=3.12

\* (cheminf is the name of the new environment, we recommend that you use the same)

### Write: y

### Then activate it, typing:

conda activate cheminf

\* (To deactivate an active environment, use conda deactivate)

## Install the course libraries in your new environment. (15 min)

### With the environment activate, enter the following commands separately. Note some installations may take a few minutes. If you run into any issues, try to install the module using pip.

conda install ipykernel

conda install -y -c conda-forge openbabel=3.1.1

conda install -y -c conda-forge xtb=6.7.1

pip install aqme

pip install robert

conda install -y -c conda-forge glib

conda install -y -c conda-forge gtk3

conda install -y -c conda-forge pango

### Install the code accelarator for ROBER (only if your system is compatible).

### pip install scikit-learn-intelex==2025.2.0

1. Downloading Workshop Materials (when available)

### Download the files needed for these lessons.

### Create a folder called ’ML\_course’ on your Desktop.

### Move the downloaded materials to the new folder.

### Unzip the file.

1. How to use Jupyter Notebook and check the set up

### Search and run Anaconda Navigator in the Windows Start.

### Lunch Jupyter Notebook.

### You will find a screen below when you run Jupyter Notebook.

Interfaz de usuario gráfica, Aplicación, Correo electrónico

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### Find your Desktop, and then go to the folder ’ML\_course’ created before.

## Checking the set up

### Double-click the course\_setup.ipynb file.

\* (.ipynb means Interactive Python Notebook)

### Go to Kernel 🡪 Change Kernel, and select the option **Python [conda env:cheminf]**

Interfaz de usuario gráfica, Texto, Aplicación

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### Run each cell by placing the cursor on each cell an pressing the play button or *Shift key* + *Enter*

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### Check that each cell indicates that the library or program have been installed correctly.

# Checking the CSV files

## A **CSV (Comma-Separated Values)** file is a simple text file used to store tabular data, where each line represents a row and values are separated by commas. It's commonly used for exchanging data between programs like spreadsheets and databases.

## Possible errors when working with CSV files:

Try to open a CSV file from the course folder.

If when opening a CSV file everything is condensed into a single column, you can change this in **Control Panel 🡪 Region 🡪 Additional Settings 🡪 In the list separator, put a ,**.

Moreover, in Excel to change the decimal separator in **File 🡪 Options 🡪 Advanced, and in the “editing options” section (first one), uncheck the “use system separators” and change the decimal separator to a period instead of a comma**. You can erase the thousand separator. Then click ok, and the settings should have changed so that the .csv files function correctly.