Create a new environment within Python (Python version 3.10 is recommended for compatibility with package dependencies).

Make sure that you have Matlab installed on your machine before proceeding further.

Install matlab.engine with pip install matlab.engine (needed for running the adhesive bonding simulator code). Make sure that the versions of Python, Matlab, and Matlab.enginge are compatible!

A screenshot of a computer

Description automatically generated

Try to run the optimize\_toy.py script now.

If you get an error that sounds like the following: “AttributeError: 'UniformFloatHyperparameter' object has no attribute ‘q’", then try to downgrade the ConfigSpace package with pip install ConfigSpace==0.7.1 (a version of that package that is compatible). Hopefully by now you will be able to run the optimize\_toy.py script without errors.

Try to run the analysis of one of the materials in the script ctpe\_x\_bonding\_model.py, perhaps lowering the n\_macroreps variable to 1 or 2. If you get an error complaining on the “ax” package, try to install “ax”. You may encounter issues with “graphql-core<3” “graphql-relay<3” “graphql-ws<0.3”. Downgrade pip with pip install pip==20.3.4 run in cmd (I open it up from anaconda. See below. Note you need to choose your environment).A screenshot of a computer

Description automatically generated

Afterwards, run this: pip install "graphql-core<3" "graphql-relay<3" "graphql-ws<0.3".

pip install ax

ERROR: Could not install packages due to an EnvironmentError: [WinError 5] Access is denied: 'C:\\Users\\piecu\\anaconda3\\envs\\ctpe\_final\\Lib\\site-packages\\~qlalchemy\\cimmutabledict.cp310-win\_amd64.pyd'

Consider using the `--user` option or check the permissions.

Running the pip install ax with admin rights should help.

Now running optimize\_toy.py will throw an error:

ModuleNotFoundError: No module named 'hypermapper'

Fix it with the following:

pip install git+https://github.com/luinardi/hypermapper.git

Installation of hypermapper crashes. Need to upgrade/downgrade setuptools.

Successfully installed setuptools-75.6.0 (didn’t work)

pip install setuptools==58.0.4 (this worked)

pip install git+https://github.com/luinardi/hypermapper.git