Technical University of Munich

ROSTLAB.

Chair for Bioinformatics and Computational Biology
Advanced Bioinformatics SoSe 2022
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Exercise sheet -1

Docker

We will use docker in this class to easily distribute our **testing** environment. Thus you can all run and test your code under the same conditions.
You do not have to use Docker. It is also possible to use your own setup in order to solve and more specifically test your implementation of the exercises.

Installation

The installation process of docker heavily depends on your OS. It is fairly easy for *nix based systems and a little bit more challenging for windows-based systems. We compiled a list of tutorials for the respective Operating Systems that you can follow:

- Debian/ Ubuntu: https://runnable.com/docker/install-docker-on-linux
- Windows: https://docs.docker.com/docker-for-windows/install/
- Windows Subsystem Linux 2: https://docs.docker.com/desktop/windows/wsl/
- macOS: https://docs.docker.com/docker-for-mac/install/

Run Pytest

Our docker environment ships with the same environment, we used to build and test the solution. As pytest changes a lot we recommend using our container for your local tests as well. To run pytest on docker using your local code first, open a shell and navigate into your code directory e.g. exercise0. Run:

- *nix: `docker run --rm -it -v $(pwd):/workspace/exercise registry.rostlab.org/rostlab/abi pytest -v`
- windows: `docker run --rm -it -v %cd%:/workspace/exercise registry.rostlab.org/rostlab/abi pytest -v`

You can modify the pytest command to suit your needs or substitute it through python or bash calls. Your code on the docker container will be in `/workspace`.

To update the docker image use: `docker pull registry.rostlab.org/rostlab/abi`

Install Dependencies Locally (Alternative)

If you don't want to use docker for running pytest, you can install everything locally on your machine. For this reason, we provide a `requirements.txt` file that allows to install the python dependencies. Please note that we use python 3.9.11 and will only provide support for this version.

You can install the requirements using: `pip3 install -r requirements.txt`. We recommend using virtual environments for your local installation. If you manage them using conda, you can install the packages with `conda install --yes --file requirements.txt`