CPE 486/586: Machine Learning for Engineers

02 Tools for Machine Learning

Fall 2025

Rahul Bhadani
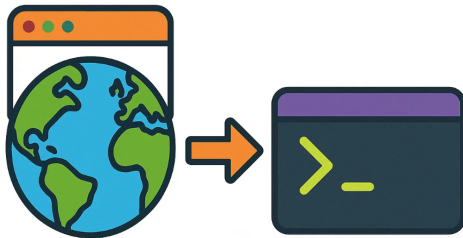
Outline

Command Line Tools and Linux

Why Command Line Tools and Linux

1. Download data from another location, webpage or server

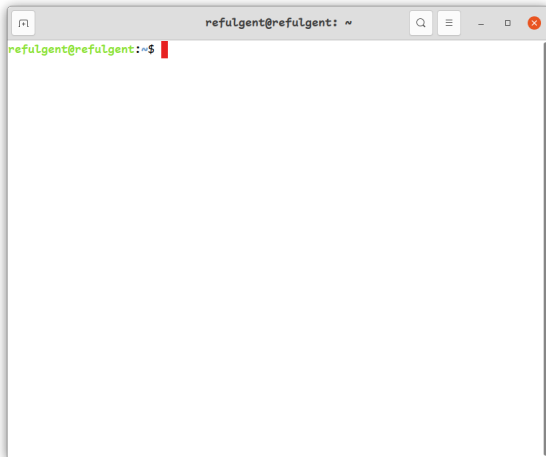# Why Command Line Tools and Linux

2. File operation, renaming, copying, editing, etc, in bulk.

3. Logging into remote server
4. To integrate with other languages and tools.
5. Command Line provides scalability, extensibility, and can automate the entire pipeline for machine learning and data science.

Command Line

1. Terminals in Linux and Macbook
2. Windows. Several Options:
   1. Git Bash. Install guide:
      https://youtu.be/SsdpuprzRE0
   2. Cygwin. Install guide:
      https://youtu.be/_j0Prs7aggo
   3. WSL.Install guide: 1.
      https://youtu.be/GMhV5Uqd8R8, 2.
      https://youtu.be/NPuIUT_6NeM?si=
      g0N39WfsBf3kIKCx

Common Linux Commands

My recommendation is to use Windows Subsystem for Linux, as it provides full linux funtionality to Windows.

A good tutorial to get started is **Getting started with Linux and Bash** at
https://learn.microsoft.com/en-us/windows/wsl/tutorials/linux

1. Installing Software:

   ```
   sudo apt-get install vim git
   ```
2. Get the working directory path:

   ```
   pwd
   ```
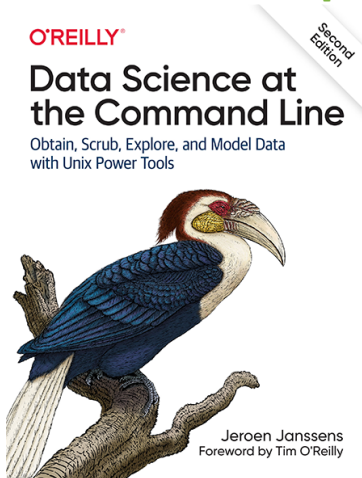3. Change directory:

   ```
   cd /data/ch02
   ```
4. Create a directory or folder:

   ```
   mkdir data
   ```

An in-depth tutorial is at

`https://jeroenjanssens.com/dsatcl/chapter-1-introduction`

Remote Logging

If you do not have a powerful machine, you can remotely logging into UAH Engineering Linux Server using your UAH ID.

```
ssh rkb0022@blackhawk.ece.uah.edu
```

Windows users should use WSL Terminals.

Python

Installing Python

Most machine learning libraries and codebase are written Python. Python is supported by a strong open-source community.

Windows users download from https://www.python.org/downloads/

Mac users download from https://www.python.org/downloads/macos/

Linux users install from command line

```
sudo apt-get install python3.12
```

or

```
sudo apt-get install python3.12-full
```

Recommended version of Python for this course is Python 3.12.

Git and GitHub

Version Controlling your Development

It is must that any of your machine learning project, and in general any coding project should use Git.

You should already have Git installed in your system through Git, otherwise install.

1. Create a GitHub account and a user name.
2. Create a new repository.
3. Clone to local machine:

```
git clone https://github.com/rahulbhadani/TestRepo TestRep
```

Commonly used Git Commands I

1. Initialize an existing local folder as a git repo.

```
git init
```

2. Add remote to your local git folder (Only needs to do once per repo).

```
git remote add origin https://github.com/rahulbhadani/TestRepo.git
```

3. Add files for commit.

```
git add . # add all files
git add somefile.txt # Add specific file(s)
```

4. Commit changes with a message before you push to the remote.

```
git commit -m "Added some files" # add a meaninful message
```

Commonly used Git Commands II

5. Push to the remote.

```
git push  # shortcut command
git push -u origin # push to a specific remote named origin
git push -u origin2 HEAD:master # push to specific origin's specific branch
```

6. Pull updates from a remote.

```
git pull  # shortcut command
git pull origin master # pull from specific remote
```

7. Git undo add before commit

```
git reset filename.txt
```

8. Git undo add after commit but before push and keep your changes

Commonly used Git Commands III

`git reset --soft HEAD~1`

Git undo add after commit but before push and unstage

`git reset HEAD~1`

Git undo add after commit but before push and discard every changes

`git reset --hard HEAD~1 # use n for undoing n multiple commits`

Development Environment

Integrated Development Environment (IDE)

Why use IDEs?

1. Provides integrated view of editor, file explorer, command lines.
2. Some IDEs provide intellisense for autocomplete.
3. IDEs are also integrate with compiler/inteprerter – one click to run your code.
4. IDEs are beautiful, rich colors and fonts over boring plain text editors.
5. Many IDEs add support for additional features such as visualization, remote log in, data wranling, etc.

VS Code

Many IDEs are available such PyCharm, Atom, VS Code.

For this course, I recommend VS Code.

Visual Studio Code

VS Code supports several extensions for Python, and other necessary tools.

Installing VS Code

Download: https://code.visualstudio.com/download
On Linux, downloaded deb file can be install at command line:

```
sudo dpkg -i code_1.103.1-1755017277_amd64.deb
```

VS Code Extension

Recommended VS Code Extension:

1. Jupyter (Microsoft)
2. Jupyter Notebook Renderers (Microsoft)
3. Python (Microsoft)
4. Pylance (Microsoft)
5. Python Debugger (Microsoft)
6. Python Environments (Microsoft)
7. Remote – SSH (Microsoft)
8. Remote – SSH: Editing Configuration Files (Microsoft)
9. Remote Explorer (Microsoft)

Connecting to Remote Machine in VS Code

When connecting to remote machine on VS Code, environment variables of the remote machine takes into effect.

To connect with `blackhawk.ece.uah.edu` from outside the Engineering building, we need VPN.

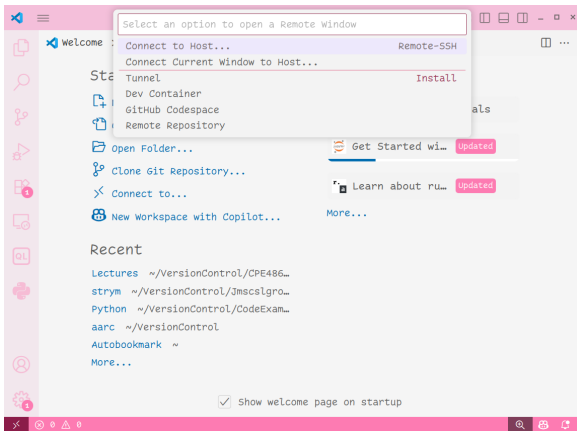Download VPN: `https://chargerware.uah.edu/all-software/secure-access-vpn`

Connecting to Remote Machine in VS Code
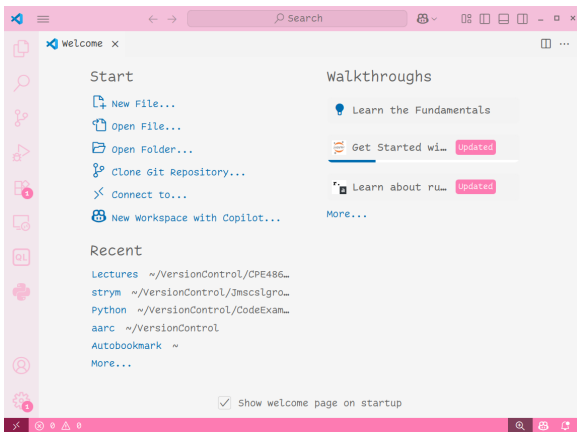
After connecting to campus VPN, click **Connect to ...**

Connecting to Remote Machine in VS Code

Click **Connect to Host ...**,
enter the address
`username@blackhawk.ece.uah.edu`. Use your own
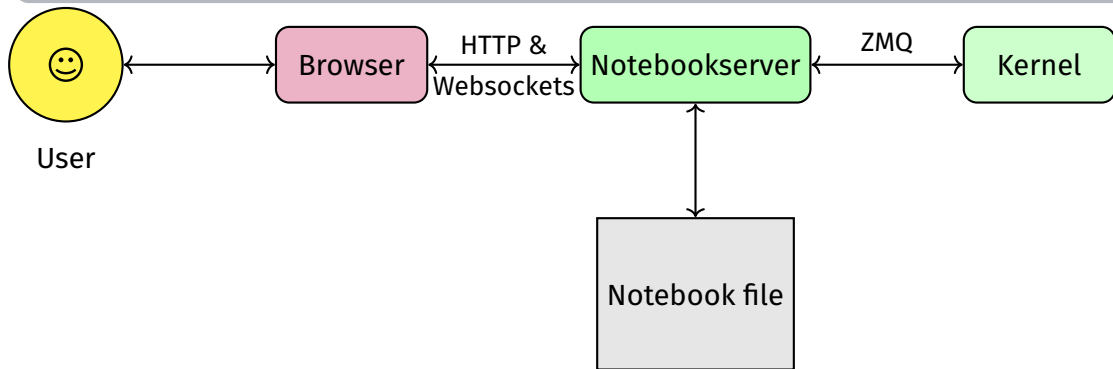user name.

Jupyter Notebook

What is Jupyter Notebook?

Jupyter Notebook is an open source web application which can be used all sorts of data science tasks. The highlight of Jupyter Notebook is reproducibilit and shareability that can combine Markdown, Latex, and plain text for documentation, comments, math, and equations, along with code. In addition, Jupyter also supports Widgets for interactivity, and provides support for multiple programming languages. Some tasks that are possible are:
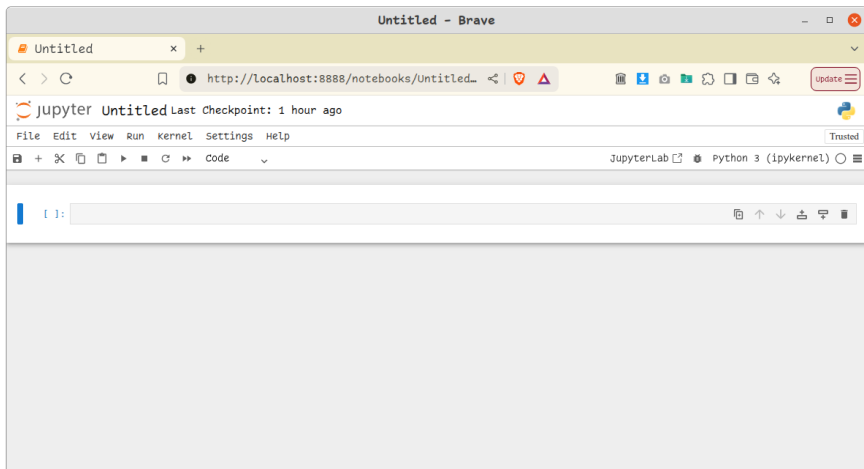
1. Data cleaning and transformation
2. Numerical simulation
3. Exploratory data analysis
4. Data visualisation
5. Statistical modeling
6. Machine learning
7. Lab notebook
8. Document sharing
9. Process documentation
10. Teaching and learning

How does Jupyter Notebook Work?

It can run locally on your own computer for lightweight use. It can also run on big servers, which we access remotely through the browser, for heavy computation.

```
   ☺                Browser    HTTP &     Notebookserver    ZMQ     Kernel
  User                        Websockets

                                    Notebook file
```

Jupyter Nootebook

Packages and Package Manager

Package / library management – Intro

⚡ Python has a vast number of packages and libraries

⚡ Installation from **official** Python Package Index
   — Always try to install from the official package manager if possible

⚡ The **pip** tool helps to find and install packages

Python Packages

⚡ Python, as a programming language, is rather lean in terms of its built-in functions.

⚡ With the help of packages, however, the range of functions can be expanded almost infinitely.

  — This is the official third-party software repository for Python.
  — It's also known as the Cheese Shop (https://youtu.be/Hz1JWzyvv8A).
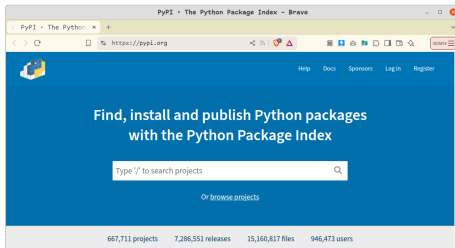

Figure: A screenshot of the Python Package Index homepage.

Python Package Tool – pip

Check your versions, you should have v3.0 for both, python & pip

Figure: Check for PIP version

Installing Python packages through PIP

```
pip install numpy # Install specific packages
```

```
pip install -r requirements.txt  # Install packages from a list of files
```

Virtual environments

1. Virtual environments isolate the version of the Python interpreter (Python binary) and all its packages in aseparated directory
2. Virtual environments are useful when you want to isolate one development activity from another, as some package versions might conflict with another versions.
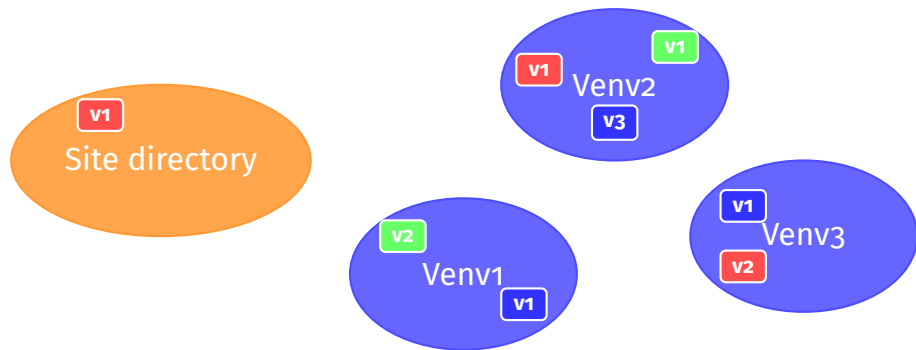
UV is a Python package and project management tool.

Once upon a time …
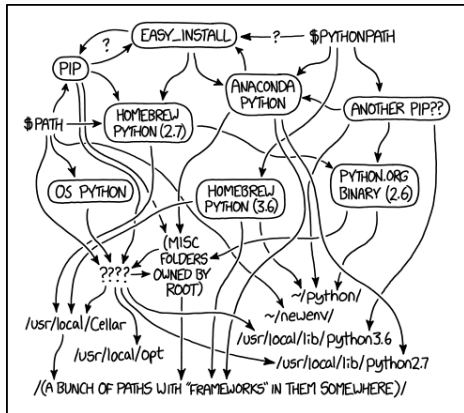
MY PYTHON ENVIRONMENT HAS BECOME SO DEGRADED
THAT MY LAPTOP HAS BEEN DECLARED A SUPERFUND SITE.

Figure: https://xkcd.com/1987/

Objectives

1. **Manage packages and dependencies:** `pip`
2. **Each project in its own environment:** `venv`, `poetry`, `hatch`, `pdm`, `rye`...
3. **Each tool in its own environment:** `pipx`
4. **Manage different Python versions:** `pyenv`

> ⚡ `uv` can potentially replace them all !!!

Limitation of `uv`

1. Not an alternative to Conda.
2. Can only install Python packages
3. However, easy to integrate with RUST programming language

Installation

1. Linux/Mac/WSL on Windows:

   ```
   curl -LsSf https://astral.sh/uv/install.sh | sh
   ```

2. Windows:

   ```
   powershell -ExecutionPolicy ByPass -c "irm https://astral.sh/uv/install.ps1 | iex"
   ```

3. Doesn't require admin rights

Python version management

1 **List installed and available Python versions:**

```
uv python list
```

2 **Install a Python version:**

```
# Install latest version
uv python install
```

```
# Install a specific version
uv python install 3.12
uv python install 3.11.10
```

Python version management

Run Python:

1. **Latest version:**

```
uv run python
```

2. **Specific version:**

```
uv run --python 3.11 python
```

3. **System version:**

```
python
```

Note:

```
uv doesn't modify the PATH.
```

Python version management

Pin a Python version in a directory:

```
# Fix default Python version
cd python_project
uv python pin 3.12
uv run python
```

If a requested Python version is not installed, `uv run` **will install it automatically:**

```
uv run --python 3.9 python
```

Remove an installed Python version:

```
uv python uninstall 3.9
```

Dependencies

Run a Python interpreter with dependencies:

```
# One dependency
uv run --with numpy python
```

```
# Several dependencies
uv run --with numpy --with matplotlib python
```

Run a command from a dependency:

```
# Launch a jupyter lab instance
uv run --with jupyterlab jupyter lab
```

```
# Launch a jupyter lab instance with numpy installed under Python 3.12
uv run --python 3.12 --with jupyterlab --with numpy jupyter lab
```

Script dependencies

Suppose we have the following `test.py` script:

```python
import numpy as np
print(np.random.rand())
```

We can run the script in a temporary virtual environment with `numpy` with:

```
uv run --with numpy test.py
```

Script dependencies

We can also add the dependency directly in the script:

```
uv add numpy --script test.py
uv run test.py
```

Dependencies have been added as inline script metadata (PEP 723):

```python
# /// script
# requires-python = ">=3.12"
# dependencies = [
#     "numpy",
# ]
# ///
import numpy as np
print(np.random.rand())
```

A script with inline metadata can be run with `uv` on any machine: required python version and dependencies will automatically be installed in a temporary virtual environment.

Projects

More complex projects must have their own persistent virtual environment.

```
# Create a project in a new folder
uv init my_project
# Create a project in the current folder
uv init .
```

uv init will:
- ⚡ create a `pyproject.toml` and a `.python-version` file
- ⚡ initialize a git repository
- ⚡ create sample `hello.py` and `README.md` files

Projects

The `pyproject.toml` file contains the project metadata and dependencies. It can be edited manually, or via `uv` commands.

```
# Add a dependency to current project
uv add numpy
# Add a dependency to current project with a minimum version
uv add "polars>=1.6"
# Add a dependency to current project with a specific version
uv add "polars==1.5"

# Remove dependency from current project
uv remove polars

# Add a development dependency
uv add --dev black
```

If your project is itself a Python package, it will be installed in the virtual environment as an editable dependency.

Projects

Dependencies constraints are resolved in the `uv.lock` lockfile.

- ⚡ `uv lock` ensures that the lockfile is still consistent with the dependencies constraints
- ⚡ `uv sync` synchronizes the virtual environment with the lockfile, installing / removing dependencies if needed

Note

- ⚡ `uv lock` and `uv sync` are automatically run after `uv add`, `uv remove` or `uv run`.
- ⚡ `uv lock` doesn't upgrade packages if new versions are available. Add `--upgrade` argument to do it.

Note

The virtual environment is created in `.venv` in the project folder. It can still be activated with `source .venv/bin/activate`.

Projects

`uv run` in a project folder (or one of its subfolders) runs the command inside the project's virtual environment.

```
# Run Python in home folder with no dependencies
cd ~
uv run python
```

```
# Run Python in a project folder. Its dependencies will be available.
cd my_project
uv run python
```

```
# Run a script in the project environment
uv run main.py
```

Projects

If an `uv` project is cloned from a git repository or copied to another machine, running `uv sync` will install the required Python version and dependencies from its `uv.lock` lockfile.

Running `uv run` to launch scripts or commands will also automatically lock the dependencies and sync the environment.

Tools

Some Python packages are installed for the application they provide:

- ⚡ `ruff`
- ⚡ `black`
- ⚡ `ipython`
- ⚡ `py-spy`
- ⚡ `snakemake`

It is highly recommended to install these tools each in their own virtual environment.

Tools

`uvx` launches a tool in a temporary environment without installing it:

```
uvx pycowsa "Hello !"
```

`uv tool` allows to install the tool in its own environment and make its binary available in the PATH:

```
uv tool add pycowsay
pycowsay "Hello !"
```

> Pay close attention to the package name when running or installing a tool. A wrong name could run a malicious command from a supply chain or typosquatting attack.

Tools

Commands to manage Python tools:

```
# List installed tools
uv tool list

# Install a tool
uv tool install radian

# Upgrade a tool
uv tool upgrade radian
# Upgrade all tools
uv tool upgrade --all

# Uninstall a tool
uv tool uninstall radian
```

Tools

(Temporary) caveats

⚡ If the default `uv` Python version is changed, tools need to be reinstalled.

⚡ Some tools need workarounds to be installed completely, for example:

```
# To install Snakemake
AR=/usr/bin/ar uv tool install snakemake
```

```
# To install Ansible
uv tool install ansible-core --with ansible
```

Markdown

Latex

Other Notable Tools

The End