

User Manual

December 5, 2021

Abstract

User Guide contains instruction for installing and running the software.

Introduction

Requirements

The software requires Python 3.8, pip, conda, git and following updated packages:

- scipy
- ProDy
- numpy
- scipy
- fuzzy-c-means
- GEM
- cdlib
- pymol
- python-dateutil
- pytz

User may install them in a conda environment or it is possible to run `install_libraries.bat` (on Windows) or `setup_macOsX.sh` on `setupLinux.sh`

Installation on Windows Platform

Windows OS: Software Installation

- 1) Check the installation of conda, python, and git.
- 2) Download and Unpack the Files.
- 3) Open a terminal window and go into the directory containing the software.
- 4) Type following commands to create a new conda environment and install all the libraries.

```
RUN setup.batinstall_libraries.bat
```

(1)

Installation on Linux Platform

Mac OS: Software Installation

- 1) Check the installation of conda, python, and git.
- 2) Download and Unpack the Files.
- 3) Open a terminal window and go into the directory containing the software.
- 4) Type following commands to create a new conda environment and install all the libraries.

```
./setupLinux.sh
```

(2)

Installation on MacOS Platform

Mac OS: Software Installation

- 1) Check the installation of conda, python, and git.
- 2) Download and Unpack the Files.
- 3) Open a terminal window and go into the directory containing the software.
- 4) Type following commands to create a new conda environment and install all the libraries.

```
./setupmacosX.sh
```

(3)

Installing Conda

Conda is a third party software for managing Python distribution. For installing conda on windows please refer to: <https://docs.conda.io/projects/conda/en/latest/user-guide/install/windows.html>

Installing git.

For git installation please refer to: <https://git-scm.com/book/en/v2/Getting-Started-Installing-Git>

Workflow of Analysis

After installing the software, in order to run it you have to open a terminal window. Then you may go into the folder in which the software is installed and type:

Launch of the Software

```
conda activate PCN
```

(4)

On Conda Prompt:

```
python pcn_main.py
```

(5)