README.md:

* Introduction
* General description and goal of the project
* Description how the code works
* Instructions on how to use and test the code + description of files
* Code (not everything)
* Limitations + suggestions for further extensions/improvements

Prerequisites/requirements.txt

* e.g. The program works with Python3
* In order to run it, the following libraries need to be installed:
* Numpy, Matplotlib, Seaborn, Sklearn, FPDF
* Editors (Spyder, VS Code, …)

Code.py

Personally I would go either with a PDF file.

Let me know what you think!