

User manual of an automatic peak deconvolution code for Raman spectra of carbonaceous materials

Shunya Kaneki

Geomechanics Research Group,
Research Institute for Geo-resources and Environment,
Geological Survey of Japan,
National Institute of Advanced Industrial Science and Technology

kaneki.shunya@aist.go.jp

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Preface

This manual explains how to run an automatic peak deconvolution code for Raman spectra of carbonaceous materials developed by Kaneki et al. (submitted to *Progress in Earth and Planetary Science*). I have tried my best to make the manual easy to understand for those unfamiliar with programming. Note that neither my institution nor myself takes any responsibility for any damage or disadvantage resulting from the use of this manual or the code.

1 Building a Python environment

Since the code was written by Python, users first need to build a Python environment in their computers. In my own opinion, this is the first big challenge that sometimes leads the beginners to give up. Such tragedy is avoidable by using a suitable software such as 'Anaconda.' Anaconda can be installed in computers operated by Windows, Macintosh, and Linux, and takes great cares of many difficulties in building a Python environment. Below I show how to build a Python environment using Anaconda. Note that depending on the policy and situations of the institution that users belong to, they need to buy licenses before using Anaconda.

1. Download 'Anaconda Installer' from an official webpage and install it.
2. Activate 'Anaconda-Navigator' and then Spyder (Figure 1).

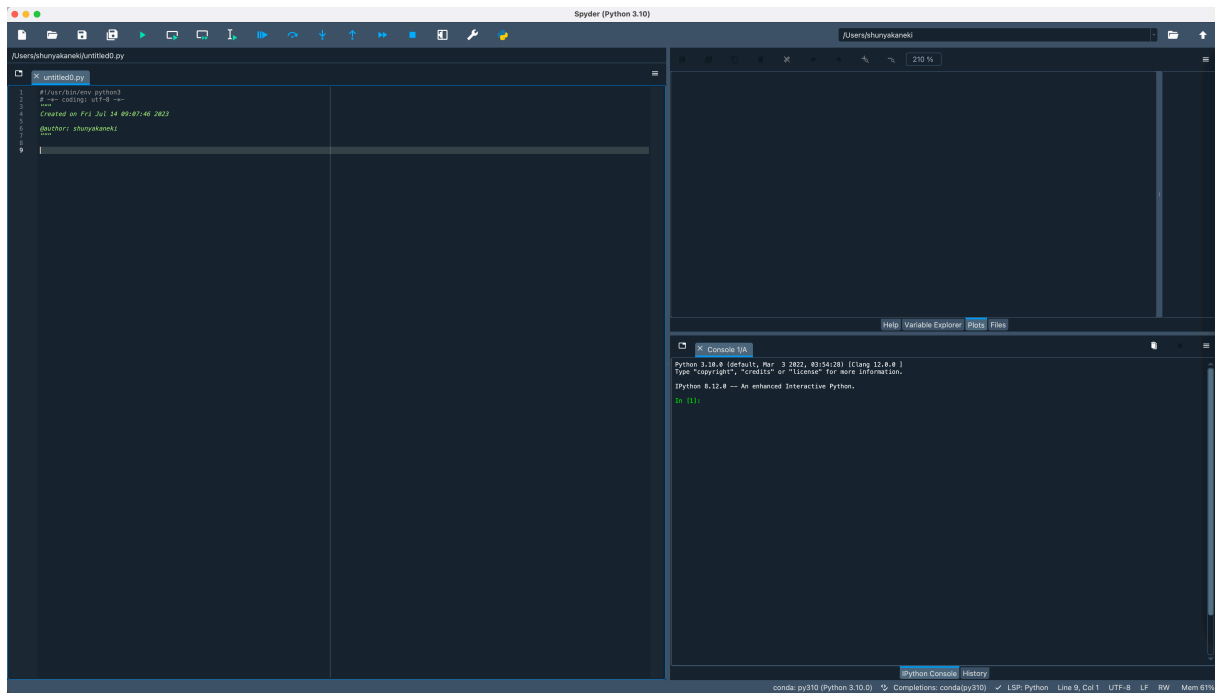
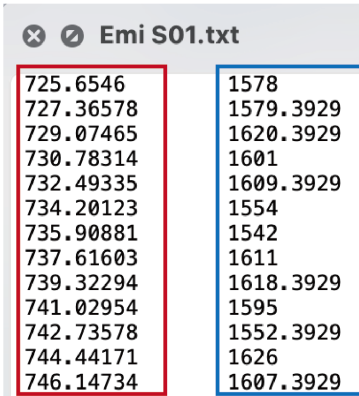


Figure 1: Screenshot of Spyder.

2 Requirement for data files of raw Raman spectra

CM Raman spectra to be processed using our code must satisfy the following two requirements (Figure 2).

- Format of the data file is either .txt, .csv, or .CSV.
- Each data file consists of two columns only of real number: first column is Raman shift in cm^{-1} and second column is intensity.



Raman shift (/cm) (1st column)	Intensity (2nd column)
725.6546	1578
727.36578	1579.3929
729.07465	1620.3929
730.78314	1601
732.49335	1609.3929
734.20123	1554
735.90881	1542
737.61603	1611
739.32294	1618.3929
741.02954	1595
742.73578	1552.3929
744.44171	1626
746.14734	1607.3929

Figure 2: Example of the Raman spectral data suitable for analysis.

3 Preparation of analytical data folder

1. Open AutoRaman_K2024 folder (Figure 3).
2. Copy AutoRaman_K2024 folder to anywhere and change its name to, for example, the sample ID. I shall call this folder as the analytical folder.
3. Copy the raw data files to the 'raw' folder in the analytical folder (Figure 4).

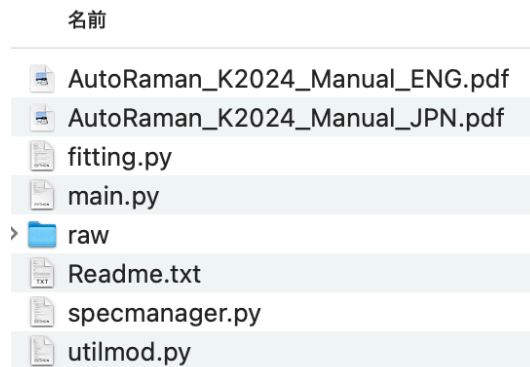


Figure 3: AutoRaman_K2024 folder.

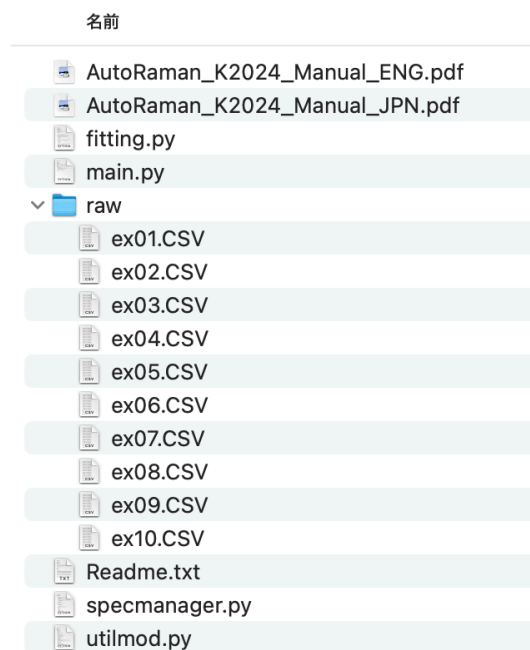


Figure 4: The analytical folder after the raw data are copied to the 'raw' folder.

4 Run the code

Run the code in Spyder.

1. Activate Spyder and open main.py in the File tab (Figure 5).
2. Change INPUT condition if necessary. 'dtype' represents the format of the raw data files and thus must be either .csv, .CSV, or .txt. **Normally, 'datadir' should not be changed.** Figures during analysis will be saved if 'figurePDF' and/or 'figurePNG' are set to True. Spectral data of the fitting results will be saved if 'specdat' is set to True.
3. Push F5 and run the code.
4. The mean temperature will be shown in the lower right window (Figure 6). When the maturity of carbonaceous materials is too low, Warning will appear to recommend to try the code of Kaneki & Kouketsu (2022).
5. In the newly made "result" folder, "image" folder saves the fitting images and histograms, "param" folder saves the initial and optimized Raman parameters, and "spec" folder saves the spectral data of the optimized spectra. "all_fin.csv" in 'param' folder saves all the Raman parameters for each spectrum. "param.csv" saves the calculated means values, standard deviation, standard error, and number of data of R1 and R2 ratios, peak positions of D1- and G-bands, and their FWHM values. "temp.csv" saves the mean, standard error, and 95% prediction interval of the maximum metamorphic temperature.
6. (Appendix) The present code performs a linear baseline correction before peak deconvolution. The spectral range during the background correction is automatically determined either 1100-1150 cm^{-1} and 1700-1750 cm^{-1} or 1200-1250 cm^{-1} and 1700-1750 cm^{-1} . If users want to change the ranges manually, change the corresponding numbers of 15-16 rows or 25-26 rows in "specmanager.py."

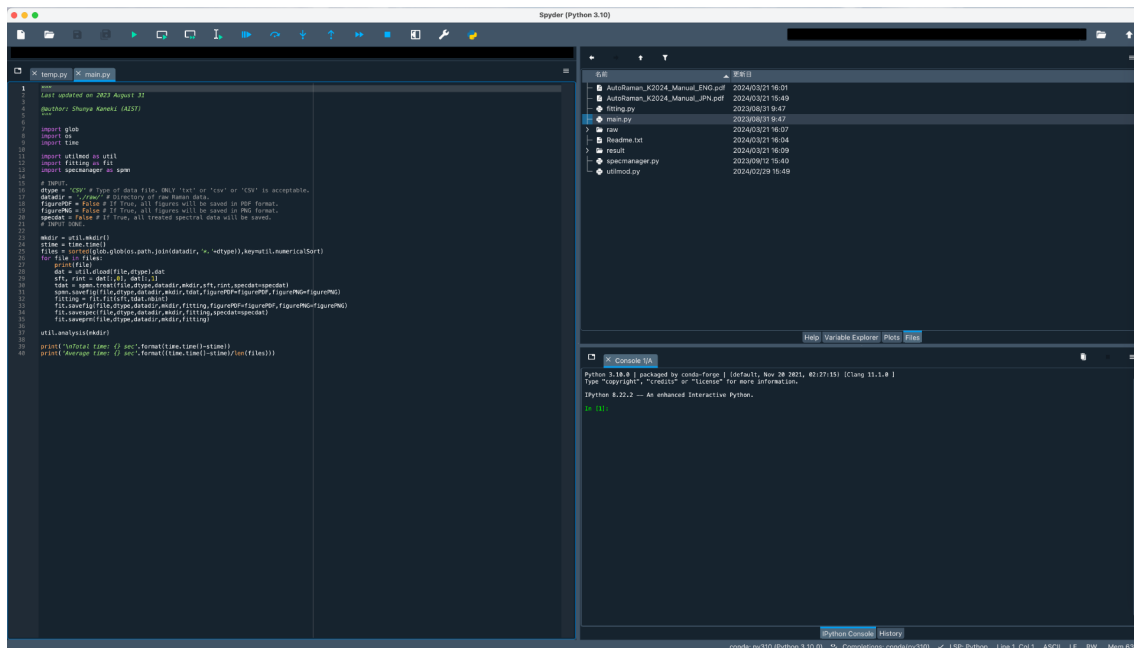


Figure 5: Screen shot of main.py.

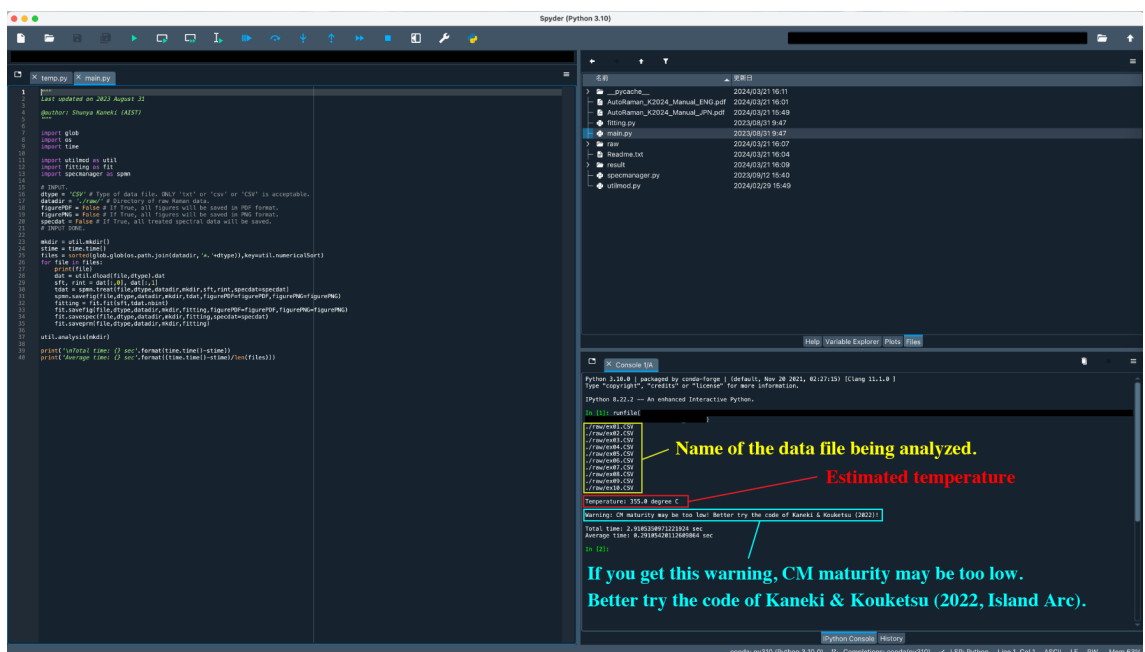


Figure 6: After analysis.