

## Workflow

### Notes:

Please download all files at [hujie802/Unmixing\\_python \(github.com\)](https://github.com/hujie802/Unmixing_python)

The ***bold and italic text*** represents the name of the folder, the **bold text** denotes the name of the code.

The date is used in naming files; keep it consistent in all codes.

- 1) Download the BayesMixQt. Check File: “**Accessing QTQt and BayesMixQt for Windows or Macintosh.pdf**” to get the software.
- 2) Follow the manual of BayesMixQt and use it to extract the signal of Zircon U-Pb data from rivers and basin.
- 3) Download Python interpreter. Anaconda is recommended. Because some packages have been updated, the old version is preferred to make the code work well. The Anaconda3-2019.07 is recommended here. The download link is [Index of / \(anaconda.com\)](#). After installing Anaconda, open Spyder (it's could be found at “Start Menu”) and use it to run the code.
- 4) Take out the necessary information from BayesMixQt result file. For river data, put BayesMixQt result files and Zircon U-Pb data for all rivers in the folder ***Extract\_results\_from\_BayesMixQt/Rivers*** and run **Extract\_results\_from\_BayesMixQt.py** to get the values of the Max Posterior Model. The values will be saved in an MS Excel file whose name starts with “map”. Meanwhile, the MDS, Sug, Fitted Normal Function, and Classification figures (Figure 5) will be generated.

Example Files:

Input file: **Data\_for\_river\_in\_optimization.xlsx**

Output file: **map\_3\_2.xlsx**

For basin data, change to ***Extract\_results\_from\_BayesMixQt/Basin*** and do the step 2 for basin U-Pb data.

Example files:

Input file: **basin\_use\_op\_2021\_2\_25.xlsx**,

Output file: **basin\_map\_3\_9.xlsx**

- 5) Unmixing modelling. Copy basin Zircon U-Pb data and BayesMixQt results of rivers and basin to *Unmixing\_code* folder. And run **Batch\_main\_mpi\_random-windows.py** to get the unmixing model. The optimization results will be saved as an MS Excel file whose name includes “sqp\_random”.

Example files:

Input files: **basin\_map\_3\_9.xlsx**, **map\_3\_2.xlsx**, **basin\_use\_op\_2021\_2\_16.xlsx**

Output file: **3\_2\_sqp\_random\_basin\_use\_op\_2021\_2\_25.xlsx**

- 6) Plotting the results. Run the code **plot\_modeling\_results\_with\_error.py** to get the figures. Setting the same date, the code will automatically read the modelling results and generate and save figures 6,7,10. Then, run code **heat\_and\_scatter\_matrix.py** to get correlation matrix and scatter matrix (figure 8 and figure s2-5)