

Workflow for FITS Spectrum Analysis

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1. Constants Setup

- **response_path:** Specifies the folder path where calibration files like RMF, ARF, and background files are stored.
- **file_path:** Specifies the path to a text file containing elemental information (e.g., $K\alpha$ excitation energies, atomic numbers, element names).
- **csv_file:** Path to the output CSV file where the results (geographic coordinates and elemental ratios) are stored.
- **ignore_eraange:** Defines the energy range to ignore during spectrum analysis (e.g., $0.9 - 4.2$ keV), converted into a string format for the XSPEC `ignore()` function.

2. Loading Elemental Data

The elemental data from the provided text file (`file_path`) is read into a `pandas` DataFrame. The DataFrame contains columns for:

- Atomic numbers
- $K\alpha$ energies
- Element names

This data is used for identifying elements and calculating fluxes.

3. Initializing the CSV File

A CSV file is created if it does not already exist. The column headers include:

- **Geographical coordinates:** Latitude and longitude corner points of the region swept by the instrument (e.g., `V0_lat`, `V0_long`, etc.).
- **Elemental intensity ratios:** Ratios of the intensity of various elements relative to silicon (e.g., `o/si`, `na/si`).

4. Processing the Input Folder

The script iterates through all files in the specified folder, processing only `.fits` files.

5. Spectrum Analysis

For each `.fits` file:

- The background spectrum, RMF (Response Matrix File), and ARF (Auxiliary Response File) are loaded using the `Spectrum` class.
- The energy range specified in `ignore_eraange` is excluded from analysis using the `ignore()` function.

6. Extracting Spectrum Data

Spectrum data is retrieved:

- **Energy edges:** The energy bins of the spectrum.
- **Counts:** Observed photon counts for each bin.
- **Energy centers:** Midpoints of the bins, calculated for further analysis.

7. Peak Detection

Peaks in the spectrum are detected using the `find_peaks()` function from `scipy.signal`. The energy values of detected peaks are compared to the known $K\alpha$ energies of elements to identify corresponding peaks.

8. Elemental Flux Calculation

For each element in the input data:

- The closest detected peak to the $K\alpha$ energy of the element is identified.
- If the detected peak is close enough (within 0.5 keV of the element's $K\alpha$ energy):
 - The flux (intensity) is calculated by integrating the spectrum counts over a small energy window around the peak.
- If no valid peak is found, the element's flux is set to 0.

9. Intensity Ratio Calculation

Silicon (Si) is used as the reference element for ratio calculations:

- For each element, the ratio of its flux to the silicon flux is calculated.
- If silicon is not detected, all ratios are set to 0.

10. Geographic Data Extraction

The FITS file's header is accessed to extract the geographic coordinates (latitude and longitude) of the corner points (V_0 , V_1 , V_2 , V_3).

11. Writing Data to CSV

A row is created containing:

- Extracted geographic data.
- Calculated intensity ratios.

This row is appended to the CSV file.

12. Final Functionality

The script processes all `.fits` files in the folder one by one and appends the results to the output CSV file. The results can be accumulated from multiple runs, as the CSV file retains existing data.