UV–Vis Spectroscopy Data Processing using Python

Overview

This repository presents a **reproducible Python-based workflow** for processing and analyzing UV–Vis spectroscopy data. The pipeline covers baseline correction, signal smoothing, and automated peak detection, and is applicable to a wide range of spectroscopic datasets in chemistry.

Problem Statement

Raw UV–Vis spectra often suffer from:

- Baseline drift
- Instrumental noise
- Overlapping absorption features

These effects can obscure chemically meaningful information and reduce analytical reliability. This workflow addresses such challenges using **well-established numerical methods** commonly applied in spectroscopy and analytical data processing.

Features

- Automated baseline correction using **Asymmetric Least Squares (ALS)**
- Noise reduction via **Savitzky–Golay** smoothing
- Robust peak detection based on **signal prominence**
- Export of detected peak positions and intensities
- Clean, publication-style visualization

Methodology

1. Data Input

- CSV file containing:
    - Column 1: Wavelength (nm)
    - Column 2: Absorbance (a.u.)

2. Baseline Correction

- **Asymmetric Least Squares (ALS)** algorithm
- Effectively removes background drift without distorting peak shapes

3. Signal Smoothing

- **Savitzky–Golay filter** applied to baseline-corrected data
- Preserves spectral features while reducing noise

4. Peak Detection

- Peaks identified using **SciPy's find_peaks**
- Detection criteria include:
    - Relative prominence
    - Minimum peak separation

5. Output

- Text file containing detected peak wavelengths and absorbance values
- Processed UV–Vis spectrum with annotated peak positions

Applications

- UV–Vis spectroscopy data preprocessing
- Educational and research-oriented spectroscopy workflows

Requirements

- Python 3.x
- NumPy
- Pandas
- SciPy
- Matplotlib

Data Ethics & Usage

- This repository contains Python scripts for data analysis developed as part of my learning and research activities. For confidentiality and proprietary reasons, **original experimental data are not shared online**. All example data included here are **simulated, anonymized, or publicly shareable**.
- No unpublished, proprietary, or supervisor-owned experimental data are included.

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Disclaimer

This code is intended for academic and research purposes. Users should adjust processing parameters according to their specific experimental conditions.